Parameterizing the binding properties of dissolved organic matter with default values skews the prediction of copper solution speciation and ecotoxicity in soil.

Supplemental Data

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Table S1. Source of trace elements and general information on the 55 soil samples

N° soil	Geographical origin	Soil type [a]	Notes and references
High geochemical background			
1	Mainland France	Colluvic cambisol	[1]
2	Mainland France	Colluvic cambisol	[1]
3	Mainland France	Cambisol	[1]
4	Mainland France	Silty-sandy, acidic [b]	[2]
5	Mainland France	Eutrophic [b]	[2]
6	Mainland France	Stagnic cambisol	[1]
7	Mainland France	Leptosol	[1]
8	Mainland France	Leptosol	[1]
9	Mainland France	Calcaric cambisol	[3]
10	Mainland France	Stagnic luvisol	[4]
11	Mainland France	Fluvic cambisol	[1]
12	Mainland France	Hypereutric cambisol	[1]
13	New Caledonia	Ferralsol	[5]

[a] According to the World Reference Base for Soil Resources 2006 [12], except for samples with b as superscript

Table S1. Continued from previous page

N° soil	Geographical origin	Soil type [a]	Notes and references
14	New Caledonia	Ferralsol	[5]
Contamination by atmospheric fallout from a former Zn-smelter plant			
15	Mainland France	Eutric cambisol	[6]
16	Mainland France	Eutric cambisol	[6]
17	Mainland France	Eutric cambisol	[6]
18	Mainland France	Eutric cambisol	[6]
19	Mainland France	Eutric cambisol	[6]
20	Mainland France	Eutric cambisol	[6]
21	Mainland France	Eutric cambisol	[6]
22	Mainland France	Eutric cambisol	[6]
23	Mainland France	Hypereutric cambisol	[6]
24	Mainland France	Calcaric cambisol	[6]
25	Mainland France	Hypereutric cambisol	[6]
26	Mainland France	Calcaric cambisol	[6]

[a] According to the World Reference Base for Soil Resources 2006 [12], except for samples with b as superscript

Table S1. Continued from previous page

N° soil	Geographical origin	Soil type [a]	Notes and references
Contamination by pesticides			
27	Mainland France	Stagnic cambisol	Former vineyard soil [7]
28	Mainland France	Stagnic luvisol	Vineyard soil [7]
29	Mainland France	Hyperskeletic leptosol	Vineyard soil [7]
30	Mainland France	Haplic luvisol	Former vineyard soil [7]
31	Mainland France	Calcaric cambisol	Former vineyard soil [7]
32	Mainland France	Hypereutric cambisol	Former vineyard soil [7]
33	Mainland France	Fluvisol	Cu-Cr-As-treated timber treatment site [7]
Contamination by the application of organic waste			
34	Island of Réunion	Andic cambisol	Field experiment, initial soil sample [8]
35	Island of Réunion	Andic cambisol	Field experiment, mineral fertilizer application for 9 cropping cyles [8]
36	Island of Réunion	Andic cambisol	Field experiment, mineral fertilizer application for 13 cropping cyles [8]
37	Island of Réunion	Andic cambisol	Field experiment, poultry litter compost application for 9 cropping cyles [8]

[a] According to the World Reference Base for Soil Resources 2006 [12], except for samples with b as superscript

Table S1. Continued from previous page

N° soil	Geographical origin	Soil type [a]	Notes and references
38	Island of Réunion	Andic cambisol	Field experiment, poultry litter compost application for 13 cropping cyles [8]
39	Island of Réunion	Andic cambisol	Field experiment, pig slurry compost application for 9 cropping cyles [8]
40	Island of Réunion	Andic cambisol	Field experiment, pig slurry compost application for 13 cropping cyles [8]
41	Mainland France	Dystric fluvisol	Field experiment, unfertilized for 20 years [9]
42	Mainland France	Dystric fluvisol	Field experiment, sewage sludge application for 20 years [9]
43	Mainland France	Dystric fluvisol	Field experiment, sewage sludge plus mineral N fertilizer application for 20 years [9]
44	Mainland France	Sandy fluvisol	Field experiment, urban compost plus mineral N fertilizer application for 20 years [9]
45	Mainland France	Sandy luvisol	Waste water application for ca. 100 years [10]
46	Mainland France	Sandy luvisol	Waste water application for ca. 100 years [10]
47	Mainland France	Sandy luvisol	Waste water application for ca. 100 years [10]
48	Mainland France	Sandy luvisol	Uncontaminated but same site as samples 45, 46, and 47 [10]

[a] According to the World Reference Base for Soil Resources 2006 [12], except for samples with b as superscript

Table S1. Continued from previous page

N° soil	Geographical origin	Soil type [a]	Notes and references
Unspecified contamination			
49	Mainland France	Eutric cambisol	[1]
50	Mainland France	Technosol	Artificial sandy material
51	Mainland France	Fluvic gleysol	[1]
52	Mainland France	Loamy, calcic [b]	Contaminated by industrial activities [11]
53	Mainland France	Stagnic cambisol	[1]
54	Mainland France	Loamy, calcic [b]	Contaminated by industrial activities [11]
55	Mainland France	Calcaric fluvisol	[1]

[a] According to the World Reference Base for Soil Resources 2006 [12], except for samples with b as superscript

Table S2. Physicochemical properties of the 55 soil samples[a]

N° soil	Clay[b] %	Silt[b] %	pH_{H20}[c]	$CaCO_3$[d] %	Corg[e] %	Corg/N[ef]	CEC[g] cmol/kg	Fe oxide[h] g/kg	Al oxide[h] g/kg	Total Cu[i] mg/kg
High geochemical background										
1	27	24	5.2	nd	2.7	1.0	6.0	81	36	26
2	21	22	5.4	nd	1.2	1.0	4.4	78	35	25
3	19	13	5.5	0.1	2.3	1.1	8.3	58	17	10
4	20	18	5.9	0.1	1.5	1.0	10.6	60	23	124
5	18	18	6.1	0.2	1.8	1.2	13.0	75	13	22
6	48	29	6.2	nd	3.7	1.0	21.1	75	20	18
7	23	23	6.6	nd	5.6	1.7	18.1	51	18	22
8	25	43	6.6	nd	2.0	1.1	13.0	81	13	17
9	40	26	7.4	1.7	3.6	1.4	22.9	55	21	237
10	26	38	7.5	1.5	2.5	1.0	32.5	205	41	42
11	26	35	7.5	nd	1.2	1.1	21.7	56	22	18
12	33	25	7.8	0.9	0.9	1.0	27.7	32	25	28

[a] $n = 55$, except for $CaCO_3$ for which $n = 14$.

[b] according to AFNOR NF X 31-107.

[c] according to NF ISO 10390.

[d] according to NF ISO 10693.

[e] according to NF ISO 10694.

[f] according to NF ISO 13878.

[g] according to AFNOR NF-X 31-130.

[h] extracted with $(NH_4)_2C_2O_4$ at pH 3 according to Tamm [13].

[i] according to NF ISO 11466.

Corg = organic C; CEC = cation exchange capacity; nd = not determined

Table S2. Continued from previous page

N° soil	Clay[b] %	Silt[b] %	pH_{H20}[c]	$CaCO_3$[d] %	Corg[e] %	Corg/N[ef]	CEC[g] cmol/kg	Fe oxide[h] g/kg	Al oxide[h] g/kg	Total Cu[i] mg/kg
13	14	54	5.0	0.3	0.1	2.5	0.1	55	16	31
14	18	25	6.1	0.4	0.2	2.4	0.6	70	15	34
Contamination by atmospheric fallout from a former Zn-smelter plant										
15	6	7	4.5	0.1	2.3	2.0	1.5	21	11	7
16	13	15	5.3	0.1	3.9	1.3	10.2	49	11	22
17	14	8	5.4	0.1	2.3	1.5	9.0	45	9	28
18	11	10	5.9	nd	1.4	1.4	5.1	26	9	24
19	11	5	5.8	nd	2.5	1.5	7.8	17	8	27
20	6	8	6.1	0.1	2.7	1.7	5.8	28	13	6
21	17	10	6.4	0.2	3.4	1.4	19.5	33	12	21
22	10	9	6.6	0.3	2.3	1.5	8.6	23	8	12
23	53	27	7.1	5.2	12.6	1.2	73.8	74	16	56
24	15	12	7.3	0.4	1.9	1.5	13.7	27	11	24

[a] $n = 55$, except for $CaCO_3$ for which $n = 14$.

[b] according to AFNOR NF X 31-107.

[c] according to NF ISO 10390.

[d] according to NF ISO 10693.

[e] according to NF ISO 10694.

[f] according to NF ISO 13878.

[g] according to AFNOR NF-X 31-130.

[h] extracted with $(NH_4)_2C_2O_4$ at pH 3 according to Tamm [13].

[i] according to NF ISO 11466.

Corg = organic C; CEC = cation exchange capacity; nd = not determined

Table S2. Continued from previous page

	Clay[b]	Silt[b]	pH_{H20}[c]	$CaCO_3$[d]	Corg[e]	Corg/N[ef]	CEC[g]	Fe oxide[h]	Al oxide[h]	Total Cu[i]
N° soil	%	%		%	%		cmol/kg	g/kg	g/kg	mg/kg
25	46	37	7.6	10.5	4.9	1.2	45.2	84	23	32
26	6	1	8.2	1.4	0.2	1.5	3.9	8	4	7
Contamination by pesticides										
27	18	33	5.5	nd	1.3	1.0	5.7	38	17	136
28	13	16	6.0	nd	0.7	1.2	3.9	20	10	94
29	12	15	6.2	nd	1.3	1.3	3.8	24	13	94
30	10	18	6.7	0.1	1.2	1.4	5.3	14	10	22
31	29	32	8.0	22.1	3.8	1.5	20.2	23	14	288
32	15	7	8.2	4.6	1.7	1.1	12.0	17	17	412
33	7	5	7.0	nd	0.7	1.4	2.8	16	9	1070
Contamination by organic waste application										
34	14	26	5.4	0.3	3.1	1.2	9.5	142	156	89
35	15	29	5.5	0.4	3.3	1.0	10.0	154	161	93

[a] n = 55, except for $CaCO_3$ for which n = 14.

[b] according to AFNOR NF X 31-107.

[c] according to NF ISO 10390.

[d] according to NF ISO 10693.

[e] according to NF ISO 10694.

[f] according to NF ISO 13878.

[g] according to AFNOR NF-X 31-130.

[h] extracted with $(NH_4)_2C_2O_4$ at pH 3 according to Tamm [13].

[i] according to NF ISO 11466.

Corg = organic C; CEC = cation exchange capacity; nd = not determined

Table S2. Continued from previous page

	Clay[b]	Silt[b]	pH_{H20}[c]	$CaCO_3$[d]	Corg[e]	Corg/N[ef]	CEC[g]	Fe oxide[h]	Al oxide[h]	Total Cu[i]
N° soil	%	%		%	%		cmol/kg	g/kg	g/kg	mg/kg
36	15	30	5.3	0.3	3.3	1.0	10.1	153	166	94
37	9	26	6.1	0.4	3.4	1.0	16.7	149	161	94
38	7	25	6.3	0.4	3.5	1.0	19.3	159	167	95
39	9	27	6.3	0.4	3.9	1.0	19.0	150	153	100
40	6	25	6.7	0.5	4.2	1.1	23.3	139	147	120
41	4	3	6.3	0.0	0.8	1.4	2.3	5	2	14
42	3	6	6.5	0.0	1.0	1.3	2.6	5	2	26
43	4	2	5.5	0.0	1.3	1.4	2.1	6	3	24
44	4	4	6.0	0.0	1.4	1.4	3.0	7	3	25
45	9	8	6.9	4.5	3.6	1.9	8.7	55	11	367
46	8	6	7.2	0.9	4.9	2.3	10.8	41	12	234
47	16	5	7.7	6.6	1.3	1.2	11.4	22	11	98
48	9	3	7.9	1.6	1.1	1.5	7.5	10	7	9

[a] $n = 55$, except for $CaCO_3$ for which $n = 14$.

[b] according to AFNOR NF X 31-107.

[c] according to NF ISO 10390.

[d] according to NF ISO 10693.

[e] according to NF ISO 10694.

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[h] extracted with $(NH_4)_2C_2O_4$ at pH 3 according to Tamm [13].

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Corg = organic C; CEC = cation exchange capacity; nd = not determined

Table S2. Continued from previous page

N° soil	Clay[b] %	Silt[b] %	pH_{H20}[c]	$CaCO_3$[d] %	Corg[e] %	Corg/N[ef]	CEC[g] cmol/kg	Fe oxide[h] g/kg	Al oxide[h] g/kg	Total Cu[i] mg/kg
Unspecified contamination										
49	23	24	4.4	nd	1.7	1.4	4.8	40	27	17
50	8	8	6.4	1.7	11.0	3.1	14.7	52	23	280
51	36	28	6.5	nd	0.9	0.9	20.9	106	28	27
52	26	32	7.9	11.1	1.6	1.0	22.4	18	22	38
53	19	23	8.0	0.1	1.8	1.4	14.4	28	12	20
54	17	35	8.1	5.0	3.4	1.9	18.7	29	21	73
55	13	12	8.1	13.0	3.2	1.4	15.1	15	8	18

[a] $n = 55$, except for $CaCO_3$ for which $n = 14$.

[b] according to AFNOR NF X 31-107.

[c] according to NF ISO 10390.

[d] according to NF ISO 10693.

[e] according to NF ISO 10694.

[f] according to NF ISO 13878.

[g] according to AFNOR NF-X 31-130.

[h] extracted with $(NH_4)_2C_2O_4$ at pH 3 according to Tamm [13].

[i] according to NF ISO 11466.

Corg = organic C; CEC = cation exchange capacity; nd = not determined

Table S3. *p-value* determined from Wilcoxon test performed with Statistica (version 6, StatSoft) between the 55 soil solutions of experiments 1, 2, 3, and 4 for pH, total Cu concentration (pCu_T), dissolved organic matter concentration (DOM) and Cu^{2+} activity (pCu^{2+}) [a].

Variables	Experiments	1	2	3	4
pH	1				
	2	1.39E-03			
	3	6.12E-10	7.81E-07		
	4	7.96E-07	0.09	2.53E-05	
pCu_T	1				
	2	0.46			
	3	1.04E-03	0.17		
	4	0.01	2.26E-04	2.98E-07	

[a] $n = 55$ for each variable
Significantly different at $p < 0.05$.

Table S3. Continued from previous page [a]

Variables	Experiments	1	2	3	4
log DOM	1				
	2	2.16E-05			
	3	1.20E-08	0.02		
	4	0.82	1.90E-04	2.19E-07	
pCu^{2+}	1				
	2	3.06E-10			
	3	1.17E-11	1.20E-05		
	4	3.43E-04	9.83E-06	5.32E-10	

[a] $n = 55$ for each variable
Significantly different at $p < 0.05$.

Table S4. Chemical properties of the 55 soil solutions of experiments 1, 2, 3 and 4 [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
1	**1**	6.0	8.5	17.7	9.8	27.4	1610.0	0.8	519.0	1.69	1.19	1.35	0.89	0.02	0.59	5.91	0.69	16.8
	2	5.9	8.5	14.2	7.1	15.7	1330.0	0.4	115.0	1.84	0.97	1.42	0.80	0.01	0.13	6.02	0.64	10.0
	3	6.3	9.1	33.0	22.3	5.1	185.0	3.7	4180.0	2.04	1.05	1.49	0.62	0.04	0.41	5.98	0.68	46.8
	4	6.5	9.2	129.0	10.2	4.2	38.9	1.1	201.0	1.90	0.94	1.65	0.67	0.13	0.16	5.93	0.70	18.5
	5	6.5	9.5	38.1	0.7	17.8	499.0	0.4	44.9	1.90	0.99	1.53	0.79	0.15	0.24	5.75	0.72	17.1
	6	6.5	9.4	43.1	21.6	4.5	54.0	0.9	2670.0	2.52	1.13	1.05	0.44	0.02	0.05	5.82	0.75	18.7
	7	6.6	9.3	10.1	0.1	91.9	910.0	0.3	14.3	0.98	0.95	1.61	1.54	0.02	0.01	5.61	0.71	14.1
	8	6.4	9.5	14.6	0.6	84.6	3870.0	0.0	17.5	1.16	1.19	1.51	1.70	0.02	0.01	6.13	0.74	10.4
	9	7.2	9.5	137.0	0.9	3.5	17.2	0.8	72.5	1.96	1.01	0.82	1.00	0.01	0.01	5.35	0.67	17.9
	10	7.1	9.6	21.9	0.3	3.8	18.0	0.0	60.2	2.97	1.26	1.44	0.35	0.18	0.11	6.18	0.74	14.4
	11	6.5	9	8.8	0.1	20.2	136.0	0.0	20.0	1.04	1.27	0.47	1.88	0.01	0.01	5.81	0.73	9.2
	12	7.4	9.5	16.4	0.0	12.7	18.8	0.0	13.8	2.78	1.07	0.59	0.59	0.01	0.01	6.00	0.75	13.7
	13	6.3	9.4	4.3	0.0	188.0	21.0	0.2	58.6	1.81	1.02	1.98	0.71	0.25	0.02	5.80	0.63	9.9
	14	6.5	9.3	1.1	0.0	360.0	439.0	0.0	63.4	1.68	1.07	1.99	0.61	0.15	0.02	6.12	0.27	9.0
	15	5.8	9.8	77.3	2100.0	14.3	115.0	23.5	4030.0	1.85	1.06	1.97	0.75	0.28	0.21	5.83	0.74	47.0

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
1	**16**	6.3	9.6	170.0	109.0	18.7	145.0	16.0	21300.0	1.87	1.24	1.48	0.57	0.22	0.89	5.69	0.79	63.2
	17	6.2	9.6	85.4	227.0	15.5	132.0	13.0	6860.0	1.64	1.15	1.81	0.61	0.19	0.76	5.63	0.73	66.9
	18	6.3	8.6	111.0	130.0	6.5	78.3	2.9	22700.0	1.83	1.03	1.83	0.73	0.16	0.18	5.86	0.73	21.7
	19	6.5	9.4	136.0	81.8	10.3	50.5	8.3	13300.0	1.81	0.99	1.52	0.57	0.01	0.35	5.57	0.72	32.1
	20	6.7	10.2	60.7	88.2	22.7	19.5	8.9	110.0	1.94	1.02	1.76	0.76	0.21	0.43	5.90	0.80	45.2
	21	6.7	10.3	175.0	40.9	24.6	106.0	1.6	1270.0	2.46	0.56	1.26	0.65	0.13	0.62	6.21	0.81	57.8
	22	6.7	9.8	178.0	317.0	7.9	35.2	12.3	20000.0	2.22	1.11	1.71	0.67	0.18	0.09	5.90	0.73	24.9
	23	7.4	10.5	314.0	79.2	20.0	119.0	13.2	830.0	3.04	1.10	1.09	0.31	0.18	0.86	6.05	0.89	149.5
	24	6.9	10	146.0	81.2	6.1	62.2	1.1	599.0	2.64	1.21	1.48	0.46	0.25	0.11	5.95	0.70	32.3
	25	7.6	10.6	132.0	9.2	8.2	54.3	0.1	57.7	3.16	1.09	0.64	0.39	0.18	0.13	5.50	0.71	39.6
	26	7.1	9.7	21.8	21.4	4.2	10.2	0.0	36.6	2.22	1.19	1.90	0.61	0.19	0.00	5.88	0.75	10.9
	27	6.0	6.7	790.0	11.0	9.6	281.0	0.1	314.0	1.85	1.22	1.74	0.66	0.02	0.01	5.79	0.72	10.0
	28	6.2	6.7	766.0	2.6	6.5	104.0	0.5	1080.0	1.80	1.06	1.68	0.65	0.01	0.02	5.68	0.70	8.6
	29	6.2	5.6	3730.0	9.2	6.7	208.0	7.6	4070.0	1.81	1.09	1.88	0.70	0.20	0.06	5.67	0.68	12.8
	30	6.4	7.3	710.0	1.4	6.0	31.7	0.3	320.0	1.66	1.06	1.66	0.81	0.01	0.01	5.51	0.67	61.6

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
1	**31**	7.4	9.4	356.0	0.2	5.0	3.7	0.0	40.0	2.13	0.87	1.06	1.07	0.01	0.00	5.84	0.72	16.2
	32	7.2	9.2	958.0	0.4	4.8	8.5	0.1	35.3	2.04	0.63	1.85	0.53	0.01	0.00	5.76	0.76	21.2
	33	6.5	6.3	2190.0	1.2	5.0	7.7	2.5	87.4	1.95	1.04	1.71	0.61	0.01	0.01	5.91	0.72	14.8
	34	6.2	8.7	19.8	4.1	3.8	31.7	0.0	663.0	1.66	1.27	1.77	0.68	0.24	0.21	5.80	0.46	8.6
	35	6.1	8.9	42.4	3.5	4.1	34.1	0.6	454.0	1.70	0.73	1.99	0.77	0.24	0.22	5.86	0.54	11.2
	36	6.2	9.3	31.6	4.3	5.3	27.2	0.0	412.0	1.69	1.10	2.17	0.77	0.22	0.02	6.05	0.51	11.6
	37	6.5	10.2	104.0	0.3	3.8	9.1	0.0	81.2	1.86	1.27	1.84	1.07	0.18	0.19	6.24	0.78	18.0
	38	6.5	10.3	146.0	0.3	4.5	12.9	0.0	89.8	1.78	1.19	2.03	1.08	0.16	0.01	5.97	0.77	19.5
	39	6.5	9.9	121.0	0.3	4.0	33.5	0.4	99.7	1.74	1.65	2.01	1.03	0.18	0.13	5.96	0.77	15.6
	40	6.9	10.3	169.0	0.1	4.3	7.6	0.0	47.2	1.59	1.79	2.34	1.07	0.21	0.00	5.95	0.85	26.9
	41	6.4	9.4	123.0	2.9	4.9	20.1	4.7	431.0	1.75	1.07	1.95	0.71	0.19	0.00	5.42	0.68	13.0
	42	6.5	9.5	135.0	9.3	5.3	36.5	5.2	695.0	1.75	0.73	1.94	0.72	0.10	0.01	5.34	0.69	13.2
	43	6.3	9.2	179.0	18.1	6.4	44.5	8.0	2850.0	1.69	0.96	1.86	0.71	0.14	0.01	5.39	0.69	18.2
	44	6.3	9.2	135.0	73.8	6.4	176.0	8.0	2280.0	1.71	1.19	1.87	0.71	0.16	0.01	5.50	0.69	13.4
	45	6.6	8.4	1230.0	13.6	16.9	292.0	7.3	3380.0	2.33	1.05	1.87	0.61	0.18	0.06	6.10	0.78	25.4

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
1	**46**	6.8	9.1	604.0	5.8	14.0	114.0	6.1	1210.0	2.16	1.00	1.88	0.60	0.15	0.01	6.03	0.73	24.0
	47	6.9	9.0	220.0	1.8	14.3	31.4	0.3	145.0	2.35	1.03	1.73	0.51	0.32	0.01	5.66	0.69	15.5
	48	7.0	9.7	41.9	0.5	6.5	31.6	0.0	37.9	2.24	0.87	1.94	0.69	0.14	0.00	6.05	0.75	14.4
	49	5.3	7.9	58.8	17.0	11.7	443.0	651.0	1830.0	1.62	1.02	1.54	0.74	0.01	0.12	6.03	0.71	19.5
	50	6.7	9.0	291.0	4.2	10.2	77.8	6.3	1950.0	3.08	1.10	3.18	0.73	0.15	0.05	6.73	2.04	12.7
	51	6.4	9.3	12.9	0.4	4.7	26.8	0.2	25.4	2.57	1.15	0.43	0.67	0.16	0.02	5.73	0.71	8.1
	52	7.5	9.9	89.8	11.4	5.9	21.6	59.6	15.5	3.03	0.64	0.92	0.32	0.14	0.00	5.71	0.68	16.0
	53	7.3	10.1	79.9	2.9	5.4	42.1	2.2	78.2	2.57	1.03	1.31	0.38	0.16	0.01	5.67	0.71	13.5
	54	7.3	9.7	154.0	0.8	12.4	27.5	0.9	42.4	2.52	1.28	1.63	0.49	0.19	0.01	5.95	0.72	16.3
	55	7.4	9.8	43.0	0.2	3.9	12.2	7.2	25.5	2.54	1.25	1.33	0.50	0.17	0.01	5.78	0.73	14.9

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	N-NH_4	N-NO_3	SO_4	DOM
				nM						mM								mg/L
2	**1**	6.2	8.8	47.3	8.0	28.3	1400.0	4.7	503.0	1.69	1.19	1.35	0.89	0.02	0.59	5.91	0.69	15.6
	2	5.9	8.9	25.6	7.3	16.7	1340.0	0.7	158.0	1.84	0.97	1.42	0.80	0.01	0.13	6.02	0.64	11.8
	3	6.2	9.8	35.7	21.9	4.6	190.0	3.5	4600.0	2.04	1.05	1.49	0.62	0.04	0.41	5.98	0.68	13.3
	4	6.5	9.7	91.8	14.9	2.7	47.0	0.4	353.0	1.90	0.94	1.65	0.67	0.13	0.16	5.93	0.70	16.7
	5	6.4	8.9	29.8	0.8	19.7	476.0	0.2	52.8	1.90	0.99	1.53	0.79	0.15	0.24	5.75	0.72	12.8
	6	6.4	10.2	42.6	25.5	3.9	63.4	1.2	3160.0	2.52	1.13	1.05	0.44	0.02	0.05	5.82	0.75	13.9
	7	6.7	10.4	16.5	0.6	60.5	1120.0	0.2	79.7	0.98	0.95	1.61	1.54	0.02	0.01	5.61	0.71	13.4
	8	6.4	10.3	29.2	1.2	60.8	3670.0	0.1	1510.0	1.16	1.19	1.51	1.70	0.02	0.01	6.13	0.74	12.3
	9	7.2	10.3	134.0	1.1	3.4	8.8	0.6	61.1	1.96	1.01	0.82	1.00	0.01	0.01	5.35	0.67	12.0
	10	7.3	10.4	36.7	0.3	2.9	17.8	0.0	48.8	2.97	1.26	1.44	0.35	0.18	0.11	6.18	0.74	12.0
	11	6.5	9.5	19.2	0.2	11.2	149.0	0.2	1140.0	1.04	1.27	0.47	1.88	0.01	0.01	5.81	0.73	8.3
	12	7.3	10.4	32.0	0.4	11.4	29.0	0.5	213.0	2.78	1.07	0.59	0.59	0.01	0.01	6.00	0.75	10.4
	13	6.2	9.9	11.6	0.1	379.0	17.7	0.0	34.8	1.81	1.02	1.98	0.71	0.25	0.02	5.80	0.63	7.5
	14	6.8	10	10.9	0.1	1818.5	260.0	0.1	42.3	1.68	1.07	1.99	0.61	0.15	0.02	6.12	0.27	7.0
	15	5.8	10.1	68.4	2340.0	13.0	108.0	24.3	4320.0	1.85	1.06	1.97	0.75	0.28	0.21	5.83	0.74	42.3

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	N-NH_4	N-NO_3	SO_4	DOM
				nM						mM								mg/L
2	**16**	6.3	10.1	142.0	77.9	14.4	118.0	13.4	20500.0	1.87	1.24	1.48	0.57	0.22	0.89	5.69	0.79	58.8
	17	6.4	10.9	74.5	290.0	10.3	143.0	11.7	8750.0	1.64	1.15	1.81	0.61	0.19	0.76	5.63	0.73	45.3
	18	6.4	9.2	101.0	164.0	5.4	91.3	4.0	29400.0	1.83	1.03	1.83	0.73	0.16	0.18	5.86	0.73	19.3
	19	6.5	9.5	136.0	119.0	8.9	64.7	10.3	21300.0	1.81	0.99	1.52	0.57	0.01	0.35	5.57	0.72	22.1
	20	6.8	11.4	63.1	102.0	18.0	22.8	9.2	144.0	1.94	1.02	1.76	0.76	0.21	0.43	5.90	0.80	33.5
	21	6.8	11.2	170.0	44.2	19.9	94.0	1.4	1300.0	2.46	0.56	1.26	0.65	0.13	0.62	6.21	0.81	75.0
	22	7.1	10.2	163.0	389.0	4.9	35.1	11.6	25100.0	2.22	1.11	1.71	0.67	0.18	0.09	5.90	0.73	22.6
	23	7.2	10.8	183.0	47.5	11.8	70.8	3.3	1460.0	3.04	1.10	1.09	0.31	0.18	0.86	6.05	0.89	66.0
	24	6.8	10.6	128.0	128.0	3.7	41.6	1.7	1380.0	2.64	1.21	1.48	0.46	0.25	0.11	5.95	0.70	15.0
	25	7.5	11.9	131.0	7.2	5.7	54.9	0.1	118.0	3.16	1.09	0.64	0.39	0.18	0.13	5.50	0.71	38.9
	26	7.3	9.9	32.3	18.4	2.6	11.2	0.1	45.5	2.22	1.19	1.90	0.61	0.19	0.00	5.88	0.75	7.0
	27	5.8	6.6	726.0	9.7	9.6	274.0	0.5	335.0	1.85	1.22	1.74	0.66	0.02	0.01	5.79	0.72	8.8
	28	6.2	6.5	811.0	3.2	6.4	115.0	0.7	3230.0	1.80	1.06	1.68	0.65	0.01	0.02	5.68	0.70	9.1
	29	6.4	6.4	2320.0	7.3	9.2	233.0	7.1	2960.0	1.81	1.09	1.88	0.70	0.20	0.06	5.67	0.68	26.6
	30	6.7	7.7	618.0	1.5	6.7	33.6	0.5	371.0	1.66	1.06	1.66	0.81	0.01	0.01	5.51	0.67	10.2

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	N-NH_4	N-NO_3	SO_4	DOM
				nM						mM								mg/L
2	**31**	7.5	9.8	356.0	0.2	5.3	12.9	0.2	43.3	2.13	0.87	1.06	1.07	0.01	0.00	5.84	0.72	10.2
	32	7.3	9.1	999.0	0.4	4.3	7.9	0.2	39.3	2.04	0.63	1.85	0.53	0.01	0.00	5.76	0.76	12.8
	33	6.7	6.7	1680.0	0.7	4.7	6.0	3.0	61.3	1.95	1.04	1.71	0.61	0.01	0.01	5.91	0.72	13.3
	34	6.2	9.9	36.6	5.8	3.4	35.1	0.1	732.0	1.66	1.27	1.77	0.68	0.24	0.21	5.80	0.46	10.9
	35	6.1	10	57.3	4.2	4.5	26.2	0.1	460.0	1.70	0.73	1.99	0.77	0.24	0.22	5.86	0.54	10.1
	36	6.4	10	51.8	4.1	6.0	31.8	0.1	408.0	1.69	1.10	2.17	0.77	0.22	0.02	6.05	0.51	9.7
	37	6.4	10.4	107.0	0.6	3.7	12.1	0.1	1610.0	1.86	1.27	1.84	1.07	0.18	0.19	6.24	0.78	15.6
	38	6.6	11.7	156.0	0.6	4.8	11.6	0.0	77.9	1.78	1.19	2.03	1.08	0.16	0.01	5.97	0.77	17.5
	39	6.7	10.9	123.0	0.3	3.9	7.4	0.0	101.0	1.74	1.65	2.01	1.03	0.18	0.13	5.96	0.77	17.7
	40	7.1	12.4	185.0	0.1	4.5	10.9	0.0	55.3	1.59	1.79	2.34	1.07	0.21	0.00	5.95	0.85	21.7
	41	6.6	9.8	102.0	2.8	6.1	9.3	5.5	343.0	1.75	1.07	1.95	0.71	0.19	0.00	5.42	0.68	10.4
	42	6.8	9.8	119.0	10.0	5.1	32.2	5.1	765.0	1.75	0.73	1.94	0.72	0.10	0.01	5.34	0.69	8.7
	43	6.4	9.7	143.0	12.0	5.8	29.9	7.1	1880.0	1.69	0.96	1.86	0.71	0.14	0.01	5.39	0.69	9.5
	44	6.5	9.7	157.0	57.4	5.8	130.0	8.1	1540.0	1.71	1.19	1.87	0.71	0.16	0.01	5.50	0.69	12.1
	45	6.7	8.4	912.0	14.4	13.9	279.0	6.0	3510.0	2.33	1.05	1.87	0.61	0.18	0.06	6.10	0.78	n.d

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	N-NH_4	N-NO_3	SO_4	DOM
				nM						mM								mg/L
2	**46**	6.8	9.1	485.0	7.5	12.1	116.0	5.6	1760.0	2.16	1.00	1.88	0.60	0.15	0.01	6.03	0.73	14.1
	47	7	9.1	232.0	2.3	13.3	42.3	0.4	277.0	2.35	1.03	1.73	0.51	0.32	0.01	5.66	0.69	9.3
	48	7.4	10.2	47.3	0.5	5.4	14.8	0.2	44.2	2.24	0.87	1.94	0.69	0.14	0.00	6.05	0.75	7.4
	49	5.2	7.9	68.0	17.6	12.5	419.0	797.0	1970.0	1.62	1.02	1.54	0.74	0.01	0.12	6.03	0.71	21.7
	50	6.8	9.5	279.0	3.7	9.9	69.2	10.5	1760.0	3.08	1.10	3.18	0.73	0.15	0.05	6.73	2.04	15.1
	51	6.3	10.2	32.1	2.0	6.9	34.4	0.5	165.0	2.57	1.15	0.43	0.67	0.16	0.02	5.73	0.71	10.5
	52	7.5	11	80.5	15.8	5.6	20.6	54.9	37.7	3.03	0.64	0.92	0.32	0.14	0.00	5.71	0.68	15.2
	53	7.3	10.7	75.1	4.7	6.7	30.6	1.5	111.0	2.57	1.03	1.31	0.38	0.16	0.01	5.67	0.71	13.0
	54	7.4	10.2	136.0	1.5	11.8	25.8	4.6	148.0	2.52	1.28	1.63	0.49	0.19	0.01	5.95	0.72	11.9
	55	7.5	11	79.8	1.7	4.0	19.9	9.1	1650.0	2.54	1.25	1.33	0.50	0.17	0.01	5.78	0.73	17.6

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
3	**1**	6.1	9	19.7	6.8	35.2	1280	1	377	1.69	1.19	1.35	0.89	0.02	0.59	5.91	0.69	13.6
	2	6.1	9	18.8	6.8	17.7	1260	0.8	132	1.84	0.97	1.42	0.8	0.01	0.13	6.02	0.64	10.5
	3	6.4	10.4	35.6	12.7	5.2	132	3.7	2810	2.04	1.05	1.49	0.62	0.04	0.41	5.98	0.68	12.8
	4	6.7	9.9	131	12.4	3.2	51.3	1.1	448	1.9	0.94	1.65	0.67	0.13	0.16	5.93	0.7	5.9
	5	6.6	10.2	28	0.6	26.1	512	0.3	4240	1.9	0.99	1.53	0.79	0.15	0.24	5.75	0.72	14.7
	6	6.5	11.2	49.9	21	4.8	69.8	2	3300	2.52	1.13	1.05	0.44	0.02	0.05	5.82	0.75	16.2
	7	6.7	9.9	20.9	0.6	99.7	1280	0.7	60.6	0.98	0.95	1.61	1.54	0.02	0.01	5.61	0.71	4.1
	8	6.5	10.3	21.6	0.7	93.8	4340	0.5	1620	1.16	1.19	1.51	1.7	0.02	0.01	6.13	0.74	13.2
	9	7.2	10.1	174	1.1	3.6	11.7	0.9	68.3	1.96	1.01	0.82	1	0.01	0.01	5.35	0.67	12.5
	10	7.4	10.6	156	0.4	3.1	24.9	0.1	53.6	2.97	1.26	1.44	0.35	0.18	0.11	6.18	0.74	11
	11	6.6	9.4	15.7	0.3	19.8	154	0.2	43.3	1.04	1.27	0.47	1.88	0.01	0.01	5.81	0.73	2.7
	12	7.5	10.6	25.6	0.2	12.1	32.9	0.1	38.5	2.78	1.07	0.59	0.59	0.01	0.01	6	0.75	12.8
	13	6.5	10.5	6.1	0.3	323	15.4	0.1	65	1.81	1.02	1.98	0.71	0.25	0.02	5.8	0.63	6.6
	14	6.8	10	3.6	0.1	1260.6	299.5	0.3	34.1	1.68	1.07	1.99	0.61	0.15	0.02	6.12	0.27	6.2
	15	6.1	11.1	55.4	1840	11.9	88	20.8	3320	1.85	1.06	1.97	0.75	0.28	0.21	5.83	0.74	7.6

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	N-NH_4	N-NO_3	SO_4	DOM
				nM						mM								mg/L
3	**16**	6.4	10.6	150	86.6	14	115	13.8	23700	1.87	1.24	1.48	0.57	0.22	0.89	5.69	0.79	48
	17	6.5	10.8	79.1	258	11.6	138	12.1	7650	1.64	1.15	1.81	0.61	0.19	0.76	5.63	0.73	41.3
	18	6.5	9.1	108	97.6	5.3	61.9	4.3	13900	1.83	1.03	1.83	0.73	0.16	0.18	5.86	0.73	19.2
	19	6.6	10.9	142	90.1	9.6	61.9	10.1	18300	1.81	0.99	1.52	0.57	0.01	0.35	5.57	0.72	7.9
	20	6.8	11.4	50.6	80.5	17.8	15.7	8.1	101	1.94	1.02	1.76	0.76	0.21	0.43	5.9	0.8	6.9
	21	6.9	11.6	168	35.5	17.3	92.4	1.1	29500	2.46	0.56	1.26	0.65	0.13	0.62	6.21	0.81	51
	22	7.2	10.9	183	320	5.4	35.8	15.2	22000	2.22	1.11	1.71	0.67	0.18	0.09	5.9	0.73	28.3
	23	7.4	11.6	233	55.8	14.7	86.7	4.1	516	3.04	1.1	1.09	0.31	0.18	0.86	6.05	0.89	94
	24	6.8	11.4	143	120	4.3	45.1	2.2	3170	2.64	1.21	1.48	0.46	0.25	0.11	5.95	0.7	16.9
	25	7.3	12.6	146	10.2	5.4	60.8	0.3	5990	3.16	1.09	0.64	0.39	0.18	0.13	5.5	0.71	44
	26	7.2	10.1	26.2	21.6	3.2	10.9	0.1	657	2.22	1.19	1.9	0.61	0.19	0	5.88	0.75	8.5
	27	6.3	7.2	708	8.7	12.5	265	0.3	2580	1.85	1.22	1.74	0.66	0.02	0.01	5.79	0.72	10.2
	28	6.4	6.9	889	2.9	6.7	119	0.7	1360	1.8	1.06	1.68	0.65	0.01	0.02	5.68	0.7	8.8
	29	6.3	5.9	3170	7.8	5.5	178	5.9	5650	1.81	1.09	1.88	0.7	0.2	0.06	5.67	0.68	9.1
	30	6.8	7.9	774	1.2	8.4	31.9	1.1	231	1.66	1.06	1.66	0.81	0.01	0.01	5.51	0.67	10.6

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
3	**31**	7.5	9.9	464	0.3	6.3	14.3	0.5	44.1	2.13	0.87	1.06	1.07	0.01	0	5.84	0.72	6.2
	32	7.4	9.3	1180	0.4	5.7	16.4	0.7	88.1	2.04	0.63	1.85	0.53	0.01	0	5.76	0.76	10.1
	33	6.7	6.8	2310	0.6	5.4	7.9	2.5	3770	1.95	1.04	1.71	0.61	0.01	0.01	5.91	0.72	5.9
	34	6.4	10.4	29.2	4	2.8	43.1	0.3	561	1.66	1.27	1.77	0.68	0.24	0.21	5.8	0.46	17.2
	35	6.3	10.5	48.9	3.9	4.4	21.9	0.2	2830	1.7	0.73	1.99	0.77	0.24	0.22	5.86	0.54	9.9
	36	6.3	10.4	47.7	3.4	5.9	32.4	0.2	2580	1.69	1.1	2.17	0.77	0.22	0.02	6.05	0.51	6.9
	37	6.5	11.8	111	0.3	3.6	9.2	0.3	97.1	1.86	1.27	1.84	1.07	0.18	0.19	6.24	0.78	15.4
	38	6.7	11.5	180	0.4	4.3	14.9	0.2	92.7	1.78	1.19	2.03	1.08	0.16	0.01	5.97	0.77	21.6
	39	6.7	12.2	125	0.3	2.9	9.7	0.1	68.9	1.74	1.65	2.01	1.03	0.18	0.13	5.96	0.77	16.7
	40	7.2	11.7	237	0.9	5.2	29.1	0.2	730	1.59	1.79	2.34	1.07	0.21	0	5.95	0.85	25.7
	41	6.6	10.1	103	2.7	5.6	16.5	5	3650	1.75	1.07	1.95	0.71	0.19	0	5.42	0.68	8.6
	42	6.7	10.4	159	9.5	6.1	41.8	6.1	815	1.75	0.73	1.94	0.72	0.1	0.01	5.34	0.69	9.9
	43	6.4	9.9	208	9	6.2	30.5	6.9	1570	1.69	0.96	1.86	0.71	0.14	0.01	5.39	0.69	9.8
	44	6.9	9.9	154	32.6	6.5	108	11.1	871	1.71	1.19	1.87	0.71	0.16	0.01	5.5	0.69	12.3
	45	6.7	8.4	1080	13.1	18.5	288	11.6	6250	2.33	1.05	1.87	0.61	0.18	0.06	6.1	0.78	17.7

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
3	**46**	6.9	9.3	531	6.2	13.7	111	8.9	1370	2.16	1	1.88	0.6	0.15	0.01	6.03	0.73	15.2
	47	7.2	9.9	258	2.4	16.9	48.6	0.7	682	2.35	1.03	1.73	0.51	0.32	0.01	5.66	0.69	10.5
	48	7.3	10.6	39.3	0.3	6	17.1	0.2	31.1	2.24	0.87	1.94	0.69	0.14	0	6.05	0.75	6.6
	49	5.5	8.8	59.6	16.7	12.9	397	678	1680	1.62	1.02	1.54	0.74	0.01	0.12	6.03	0.71	20.3
	50	6.9	9.7	292	3.6	10.4	66.8	7.8	1630	3.08	1.1	3.18	0.73	0.15	0.05	6.73	2.04	15.1
	51	6.6	10.3	17.5	0.5	11.7	27.4	0.4	30.4	2.57	1.15	0.43	0.67	0.16	0.02	5.73	0.71	4.6
	52	7.9	10.7	90.9	13.8	5.2	20.2	61	19.2	3.03	0.64	0.92	0.32	0.14	0	5.71	0.68	5.6
	53	7.3	10.6	80.4	6.6	8.7	38.1	3.9	120	2.57	1.03	1.31	0.38	0.16	0.01	5.67	0.71	4.2
	54	7.5	10.7	173	1.2	11.6	25.1	2.8	85	2.52	1.28	1.63	0.49	0.19	0.01	5.95	0.72	9.5
	55	7.5	12.7	53.5	0.3	3.9	16.7	8	27.8	2.54	1.25	1.33	0.5	0.17	0.01	5.78	0.73	5.3

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
4	**1**	6	9.1	17.3	8.1	24.8	1430.0	1.0	1760.0	1.69	1.19	1.35	0.89	0.02	0.59	5.91	0.69	13.9
	2	6.1	9	17.0	7.3	17.7	1320.0	1.0	142.0	1.84	0.97	1.42	0.80	0.01	0.13	6.02	0.64	8.8
	3	6.4	9.7	23.1	10.9	3.9	116.0	2.8	2470.0	2.04	1.05	1.49	0.62	0.04	0.41	5.98	0.68	38.5
	4	6.5	7.8	100.0	16.0	3.6	49.4	0.7	404.0	1.90	0.94	1.65	0.67	0.13	0.16	5.93	0.70	21.3
	5	6.5	9.4	24.0	0.5	18.3	430.0	0.2	90.8	1.90	0.99	1.53	0.79	0.15	0.24	5.75	0.72	16.5
	6	6.7	10.1	33.1	16.1	4.0	45.3	1.0	1750.0	2.52	1.13	1.05	0.44	0.02	0.05	5.82	0.75	16.7
	7	6.7	10	11.7	0.1	97.4	1160.0	0.4	122.0	0.98	0.95	1.61	1.54	0.02	0.01	5.61	0.71	14.6
	8	6.5	9.6	15.4	0.6	73.2	4020.0	0.1	22.7	1.16	1.19	1.51	1.70	0.02	0.01	6.13	0.74	11.3
	9	7.1	10.2	107.0	1.0	3.2	6.3	0.7	38.3	1.96	1.01	0.82	1.00	0.01	0.01	5.35	0.67	11.6
	10	7.3	9.6	32.0	0.3	3.0	23.9	0.2	41.2	2.97	1.26	1.44	0.35	0.18	0.11	6.18	0.74	16.1
	11	6.5	8.8	9.1	0.1	13.0	150.0	0.1	13.8	1.04	1.27	0.47	1.88	0.01	0.01	5.81	0.73	7.1
	12	7.4	10.2	14.3	0.0	9.6	22.8	0.2	9.1	2.78	1.07	0.59	0.59	0.01	0.01	6.00	0.75	10.9
	13	6.4	9.7	3.3	0.1	334.0	12.5	0.2	24.2	1.81	1.02	1.98	0.71	0.25	0.02	5.80	0.63	14.3
	14	6.7	9.5	4.4	0.0	1790.0	272.0	0.1	13.0	1.68	1.07	1.99	0.61	0.15	0.02	6.12	0.27	8.1
	15	6	9.5	67.6	2450.0	12.7	283.0	21.7	4500.0	1.85	1.06	1.97	0.75	0.28	0.21	5.83	0.74	42.0

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
4	**16**	6.4	10.3	168.0	119.0	17.3	133.0	21.6	24100.0	1.87	1.24	1.48	0.57	0.22	0.89	5.69	0.79	83.7
	17	6.3	10.1	168.0	287.0	10.5	191.0	14.0	9800.0	1.64	1.15	1.81	0.61	0.19	0.76	5.63	0.73	52.3
	18	6.3	8	90.9	181.0	5.6	107.0	4.3	36100.0	1.83	1.03	1.83	0.73	0.16	0.18	5.86	0.73	22.3
	19	6.7	9.8	159.0	107.0	13.1	68.8	12.1	19100.0	1.81	0.99	1.52	0.57	0.01	0.35	5.57	0.72	41.2
	20	6.8	10.8	52.5	78.8	18.1	16.7	8.8	419.0	1.94	1.02	1.76	0.76	0.21	0.43	5.90	0.80	43.8
	21	6.8	10.4	133.0	37.3	19.9	73.5	1.8	1090.0	2.46	0.56	1.26	0.65	0.13	0.62	6.21	0.81	37.2
	22	6.9	10.2	151.0	386.0	5.2	33.8	11.6	24500.0	2.22	1.11	1.71	0.67	0.18	0.09	5.90	0.73	74.2
	23	7.2	10.8	220.0	53.0	13.3	128.0	3.7	472.0	3.04	1.10	1.09	0.31	0.18	0.86	6.05	0.89	89.5
	24	6.9	10	167.0	137.0	3.4	535.0	2.1	1020.0	2.64	1.21	1.48	0.46	0.25	0.11	5.95	0.70	19.2
	25	7.3	11.1	123.0	7.5	5.2	53.3	0.2	51.2	3.16	1.09	0.64	0.39	0.18	0.13	5.50	0.71	39.4
	26	7.2	9.9	24.4	22.1	9.0	14.2	0.4	82.6	2.22	1.19	1.90	0.61	0.19	0.00	5.88	0.75	9.4
	27	6.1	6.6	811.0	13.2	10.1	343.0	0.4	576.0	1.85	1.22	1.74	0.66	0.02	0.01	5.79	0.72	10.1
	28	6.4	6.8	554.0	2.2	4.3	89.7	0.3	947.0	1.80	1.06	1.68	0.65	0.01	0.02	5.68	0.70	7.7
	29	6.3	5.8	2880.0	7.3	6.1	202.0	6.2	3980.0	1.81	1.09	1.88	0.70	0.20	0.06	5.67	0.68	20.6
	30	6.7	7.6	587.0	2.5	6.1	41.8	1.4	360.0	1.66	1.06	1.66	0.81	0.01	0.01	5.51	0.67	9.5

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	N-NH_4	N-NO_3	SO_4	DOM
				nM						mM								mg/L
4	**31**	7.6	9.7	374.0	0.2	6.3	8.1	0.2	14.6	2.13	0.87	1.06	1.07	0.01	0.00	5.84	0.72	13.2
	32	7.3	9.6	865.0	0.3	5.0	10.8	0.7	130.0	2.04	0.63	1.85	0.53	0.01	0.00	5.76	0.76	11.4
	33	6.7	6.5	1870.0	0.7	5.1	7.2	1.3	361.0	1.95	1.04	1.71	0.61	0.01	0.01	5.91	0.72	9.9
	34	6.3	9.6	26.3	4.4	2.8	32.5	0.3	615.0	1.66	1.27	1.77	0.68	0.24	0.21	5.80	0.46	13.0
	35	6.3	9.7	44.3	4.7	3.9	25.1	0.1	1240.0	1.70	0.73	1.99	0.77	0.24	0.22	5.86	0.54	11.7
	36	6.3	9.5	45.2	4.3	5.5	30.5	0.4	421.0	1.69	1.10	2.17	0.77	0.22	0.02	6.05	0.51	12.2
	37	6.4	10.3	97.4	0.3	4.3	8.4	0.2	81.2	1.86	1.27	1.84	1.07	0.18	0.19	6.24	0.78	25.4
	38	6.7	10.8	144.0	0.3	4.1	17.3	0.4	85.3	1.78	1.19	2.03	1.08	0.16	0.01	5.97	0.77	22.2
	39	6.6	10.7	107.0	0.3	3.8	12.0	0.2	76.0	1.74	1.65	2.01	1.03	0.18	0.13	5.96	0.77	27.5
	40	7	11.1	177.0	0.2	3.7	13.6	0.9	73.1	1.59	1.79	2.34	1.07	0.21	0.00	5.95	0.85	39.4
	41	6.9	10.4	110.0	1.5	5.4	9.3	7.8	163.0	1.75	1.07	1.95	0.71	0.19	0.00	5.42	0.68	16.3
	42	7.1	10	120.0	5.7	6.2	28.0	5.4	343.0	1.75	0.73	1.94	0.72	0.10	0.01	5.34	0.69	17.2
	43	6.6	9.9	155.0	8.9	6.6	30.9	6.5	1350.0	1.69	0.96	1.86	0.71	0.14	0.01	5.39	0.69	10.6
	44	6.9	10	141.0	36.4	8.7	96.6	11.4	822.0	1.71	1.19	1.87	0.71	0.16	0.01	5.50	0.69	20.2
	45	6.6	8.4	947.0	16.6	19.1	319.0	11.9	4490.0	2.33	1.05	1.87	0.61	0.18	0.06	6.10	0.78	20.9

Table S4. Continued from previous page [a]

Experiment	Soil	pH	pCu^{2+}	Cu	Cd	Cr	Ni	Pb	Zn	Ca	Na	K	Mg	Cl	$N\text{-}NH_4$	$N\text{-}NO_3$	SO_4	DOM
				nM						mM								mg/L
4	**46**	6.8	8.9	453.0	6.7	16.5	113.0	9.8	1570.0	2.16	1.00	1.88	0.60	0.15	0.01	6.03	0.73	19.8
	47	7.1	9.2	231.0	2.7	12.5	49.6	0.8	529.0	2.35	1.03	1.73	0.51	0.32	0.01	5.66	0.69	14.1
	48	7.1	9.6	35.3	0.2	6.0	16.8	0.2	516.0	2.24	0.87	1.94	0.69	0.14	0.00	6.05	0.75	28.7
	49	5.4	7.5	44.1	15.8	11.1	373.0	689.0	1610.0	1.62	1.02	1.54	0.74	0.01	0.12	6.03	0.71	23.1
	50	6.9	8.6	236.0	3.5	10.3	66.7	16.0	5050.0	3.08	1.10	3.18	0.73	0.15	0.05	6.73	2.04	25.3
	51	6.5	9.4	13.1	0.4	9.6	28.5	0.6	34.4	2.57	1.15	0.43	0.67	0.16	0.02	5.73	0.71	7.6
	52	7.6	8.3	73.8	17.0	4.8	20.4	51.3	17.5	3.03	0.64	0.92	0.32	0.14	0.00	5.71	0.68	11.8
	53	7.3	10.6	70.7	4.1	6.7	32.3	1.5	80.8	2.57	1.03	1.31	0.38	0.16	0.01	5.67	0.71	16.1
	54	7.4	8.9	131.0	1.0	9.7	30.0	1.0	828.0	2.52	1.28	1.63	0.49	0.19	0.01	5.95	0.72	19.8
	55	7.4	9.9	46.8	0.3	3.4	14.8	6.2	50.0	2.54	1.25	1.33	0.50	0.17	0.01	5.78	0.73	20.5

[a] DOM = dissolved organic matter; n.d = not determined

Figure S1. Measurements of pH (a), total Cu concentration (pCu_T, b), dissolved organic matter concentration (DOM, c) and Cu^{2+} activity (pCu^{2+}, d) in the 55 solutions of experiments 1, 2, 3, and 4 as a function of the mean pH, pCu_T and DOM values for the four experiments. Error bars represent the standard deviation (n = 3) for samples 18, 29, and 47. The solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 0.5 log_{10} unit.

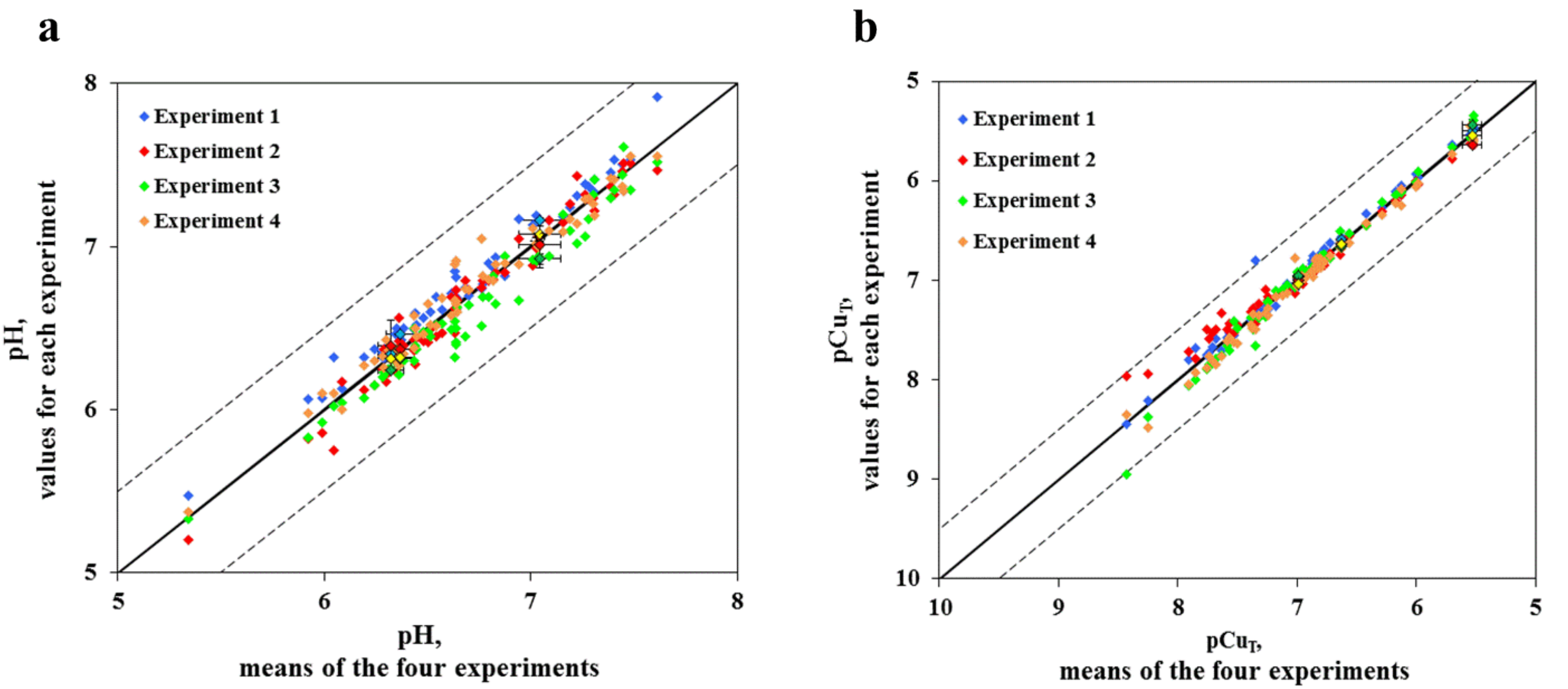

Figure S1. Continued from previous page

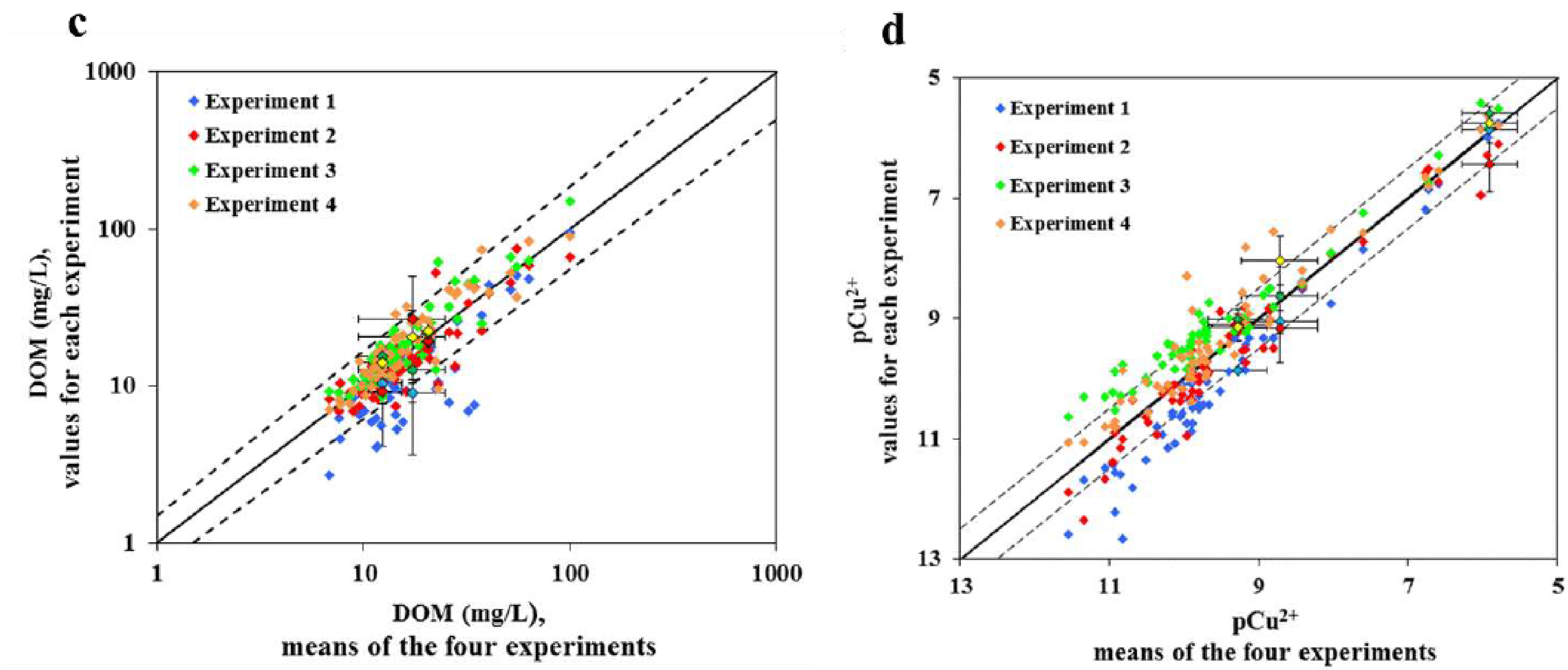

Figure S2. Optimized values for the percentage of DOM reactive towards metal cations (*% r-DOM*, a), Cu complexation constant (log K_{Cu}, b), Fe solubility products (log Ks_{Fe}, c) and Al solubility products (log K_{Al}, d) in the 55 solutions of experiments 1, 2, 3, and 4 as a function of the mean *% r-DOM*, log K_{Cu}, log Ks_{Fe} and log Ks_{Al} values for the four experiments. Error bars represent the standard deviation (n = 3) for samples 18, 29, and 47. The solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 0.5 $\log_{10}$ unit.

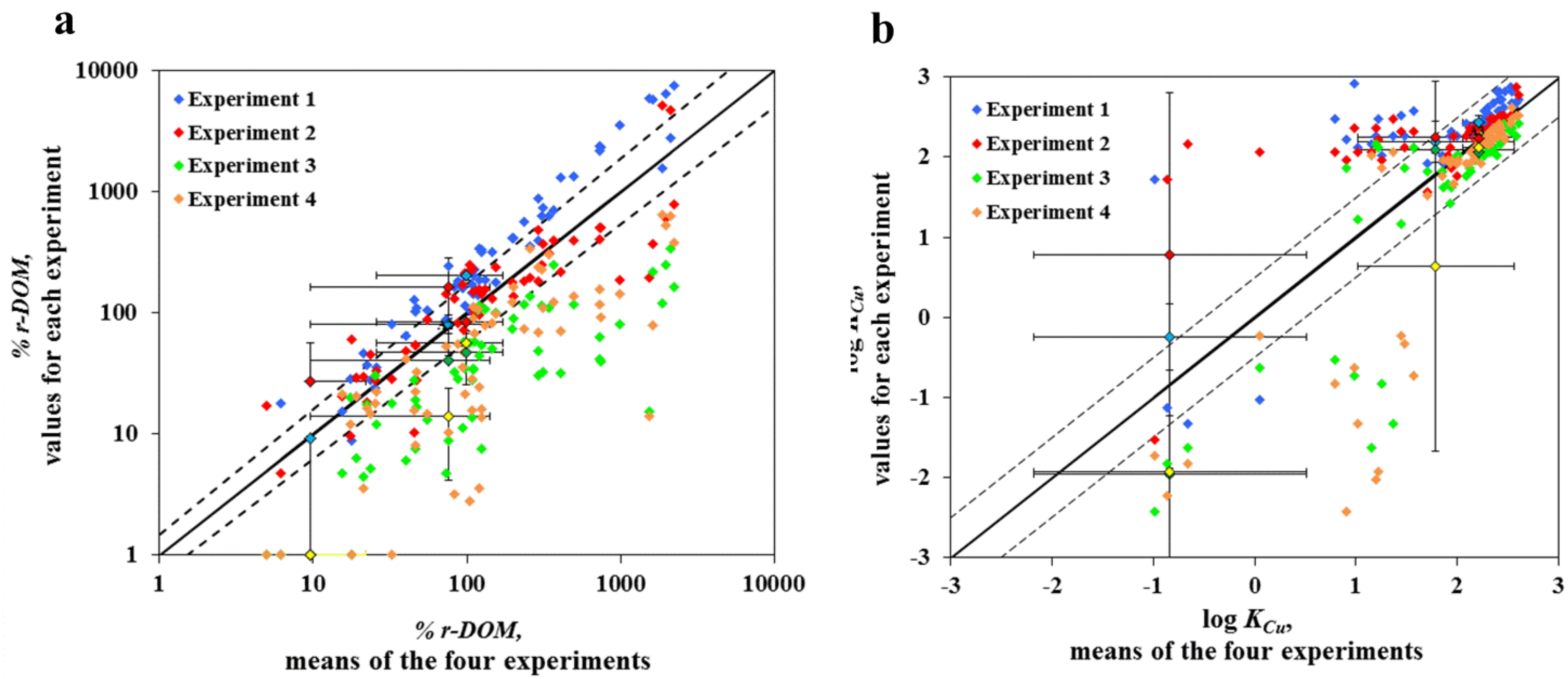

Figure S2. Continued from previous page

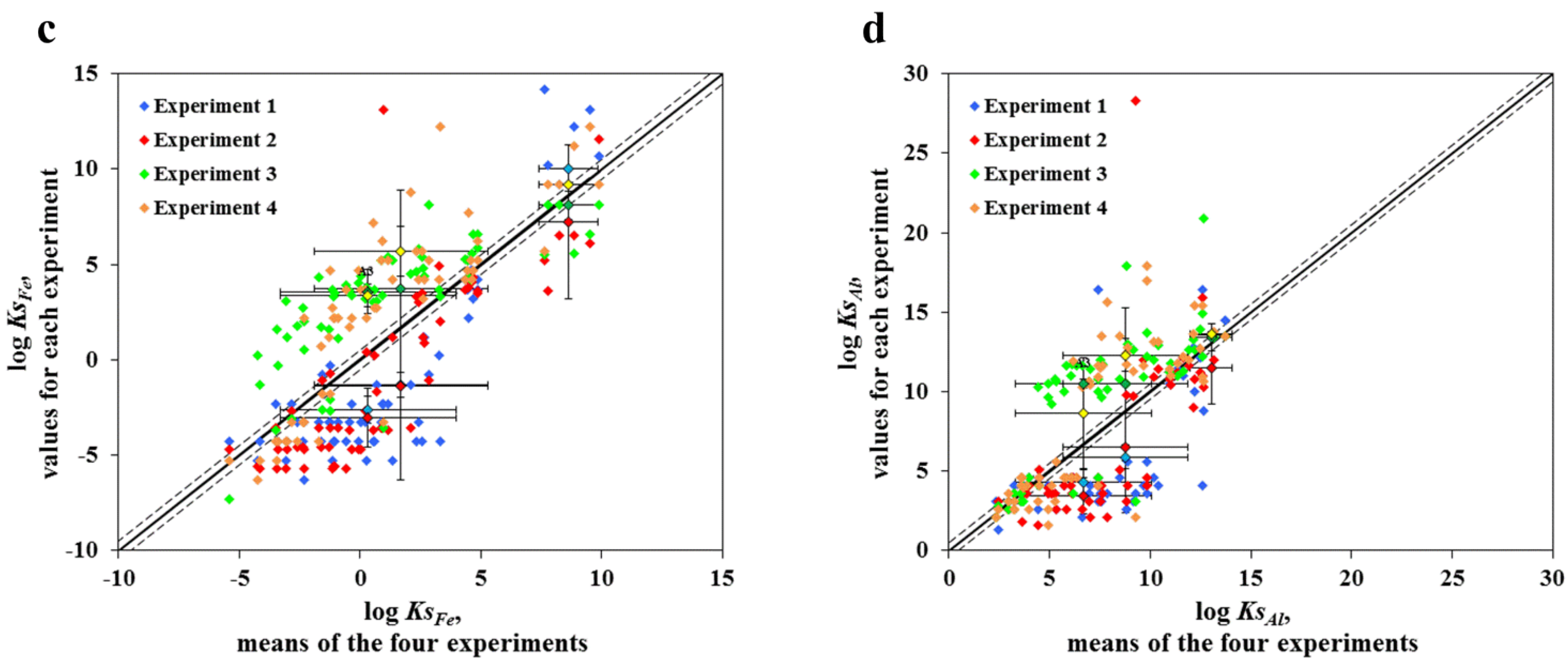

Table S5. Correlation between pH, total Cu concentration (pCu_T), dissolved organic matter concentration (log DOM) and Cu^{2+} activity (pCu^{2+}) measured in experiments 1, 2, 3, and 4 and the mean pH, pCu_T, log DOM and pCu^{2+} values for the four experiments. R^2_{adj} = adjusted R^2 [a].

Variables	R^2_{adj} in experiment 1	2	3	4
pH	0.98	0.97	0.96	0.97
pCu_T	0.98	0.98	0.99	0.99
log DOM	0.71	0.51	0.79	0.79
pCu^{2+}	0.96	0.94	0.96	0.91

[a] n = 55 for each experiment.

Table S6. Correlation between the percentage of DOM reactive towards metal cations (log *% r-DOM*), Cu complexation constant (log K_{Cu}), Fe and Al solubility products (log Ks_{Fe} and log Ks_{Al}) adjusted with WHAM VII in experiments 1, 2, 3, and 4 and the mean log *% r-DOM*, log K_{Cu}, log Ks_{Fe} and log Ks_{Al} values for the four experiments. R^2_{adj} = adjusted R^2 [a].

Variables	R^2_{adj} in experiment 1	2	3	4
log *% r-DOM*	0.83	0.78	0.78	0.79
log K_{Cu}	0.58	0.39	0.74	0.71
log Ks_{Fe}	0.75	0.69	0.55	0.71
log Ks_{Al}	0.46	0.50	0.59	0.66

[a] n = 55 for each experiment.

Table S7. Relative standard deviation between pH, total Cu concentration (pCu_T), dissolved organic matter concentration (log DOM) and Cu^{2+} activity (pCu^{2+} measured in experiments 1, 2, 3, and 4 and the mean pH, pCu_T, log DOM and log *% r-DOM* values for the four experiments [a].

Variables	Relative standard deviation (%)		
	min	mean	max
pH	0.47	1.6	4.2
pCu_T	0.34	1.2	5.1
log DOM	1.1	12.3	33.8
pCu^{2+}	0.30	5.3	12.5

[a] *n* = 55 for each experiment.

Table S8. Relative standard deviation between the percentage of DOM reactive towards metal cations (log *% r-DOM*), Cu complexation constant (log K_{Cu}), Fe and Al solubility products (log Ks_{Fe} and log Ks_{Al}) adjusted with WHAM VII in experiments 1, 2, 3, and 4 and the mean pH, pCu_T, log DOM and log *% r-DOM* values for the four experiments [a]

Variables	Relative standard deviation (%)		
	min	mean	max
log *% r-DOM*	3.3	32.8	223
log K_{Cu}	1.5	98.4	3087
log Ks_{Fe}	9.9	685	18766
log Ks_{Al}	3.0	41.7	137

[a] *n* = 55 for each experiment.

Figure S3. Metal (pCu_T, pCd_T, pNi_T, pPb_T, and pZn_T) and dissolved organic matter (DOM) concentrations, pH, and Cu^{2+}activities (pCu^{2+}) measured in the 55 soil solutions of experiments (a) 2, (b) 3 and (c) 4. The values represented from the bottom to the top indicate the minimum, first quartile, median, third quartile, and maximum values.

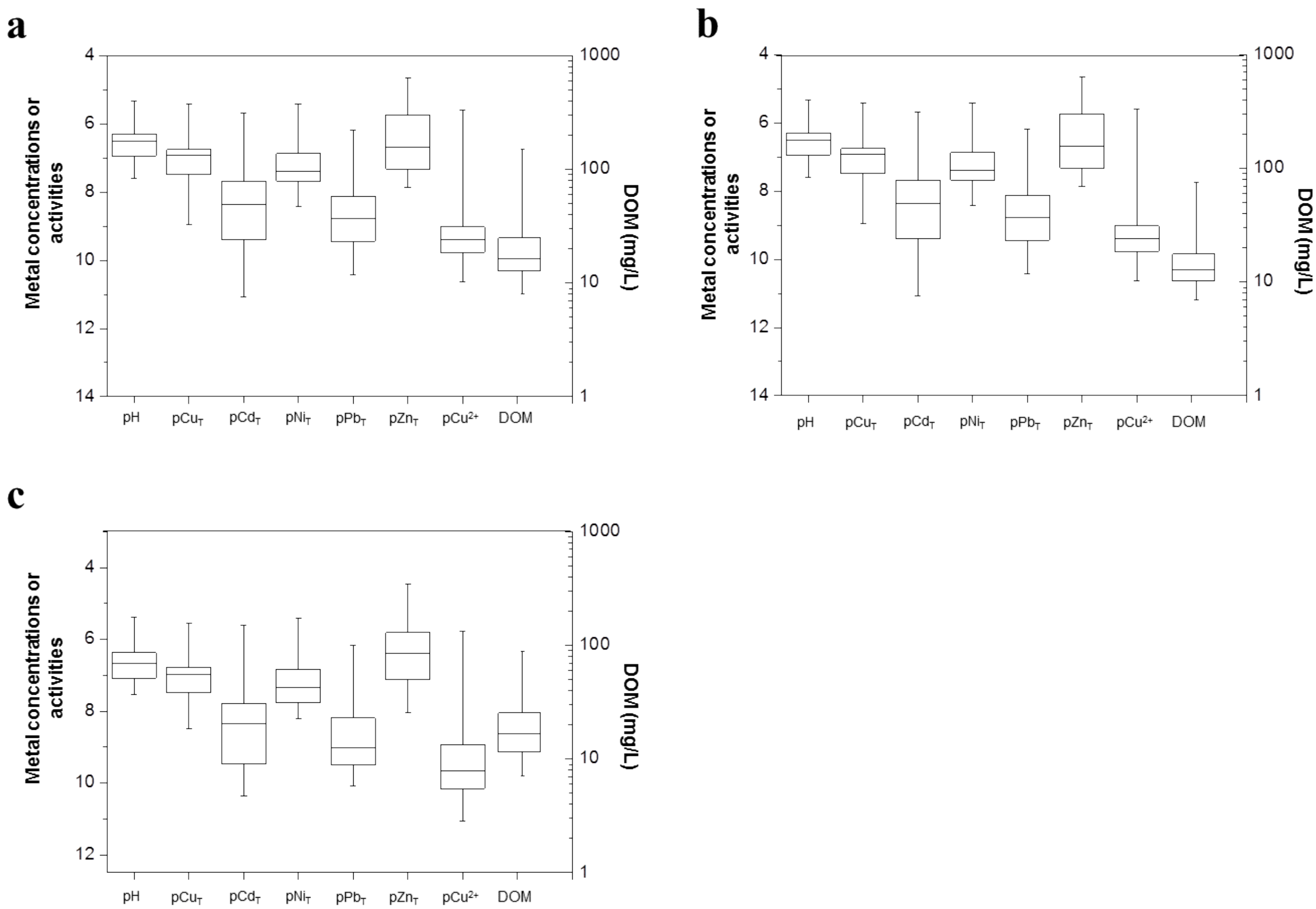

Figure S4. Free Cu activity (pCu^{2+}) predicted with WHAM VII as a function of the measured pCu^{2+} in the 55 soil solutions of experiments 2. Free Cu activity was predicted with WHAM VII by using either (a) a single, default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM* = 65 %), the Cu binding constant of reactive DOM (log K_{Cu} = 2.16), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe} = 2.7) and $Al(OH)_3$ (log Ks_{Al} = 8.5) for all solutions or (b) an optimized value of *% r-DOM* and log K_{Cu} within a range restricted to physically meaningful values for each soil solution. Vertical error bars represent the 95 % confident interval of pCu^{2+} predicted with WHAM VII when considering the analytical uncertainty on pH and total Cu and DOM concentrations (see Material and Methods section for rationale). Empty data points represent soil samples 18, 29, and 47 that were replicated thrice with their standard deviation as horizontal error bar. The thin solid line represents the regression line. The thick solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 0.5 pCu^{2+} unit. R^2_{adj} = adjusted R^2; *RMSR* = root mean square residual.

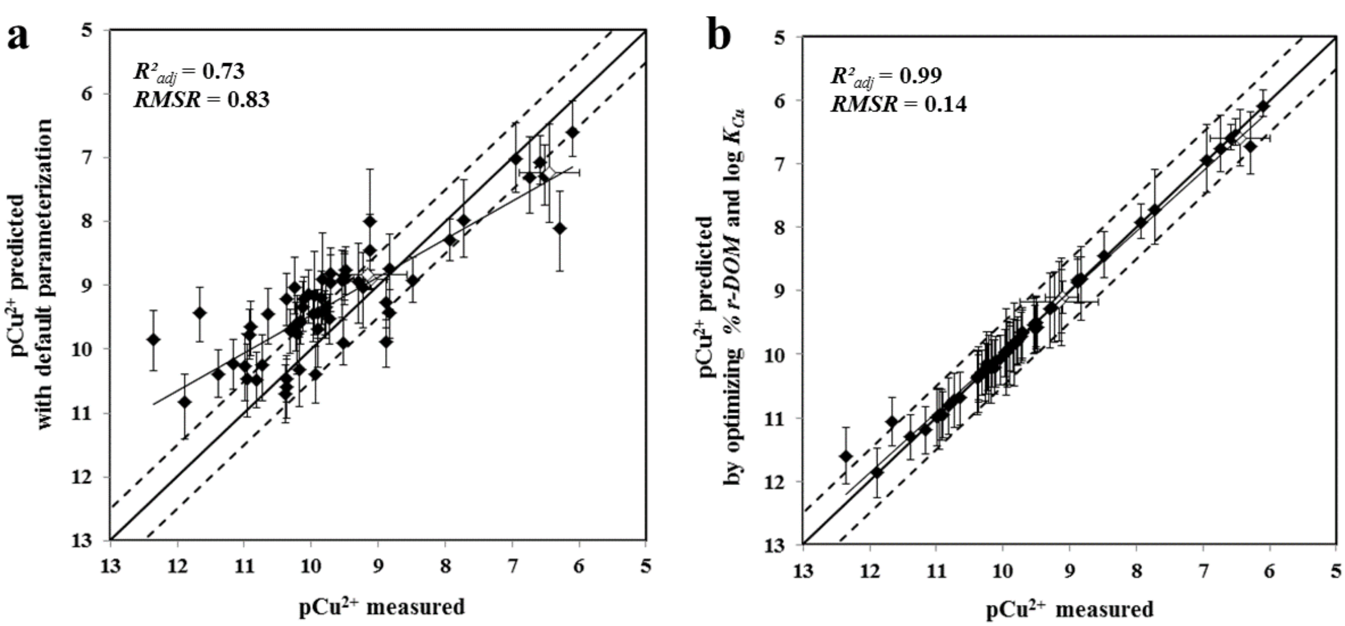

Figure S5. Free Cu activity (pCu^{2+}) predicted with WHAM VII as a function of the measured pCu^{2+} in the 55 soil solutions of experiments 3. Free Cu activity was predicted with WHAM VII by using either (a) a single, default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM* = 65 %), the Cu binding constant of reactive DOM (log K_{Cu} = 2.16), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe} = 2.7) and $Al(OH)_3$ (log Ks_{Al} = 8.5) for all solutions or (b) an optimized value of *% r-DOM* and log K_{Cu} within a range restricted to physically meaningful values for each soil solution. Vertical error bars represent the 95 % confident interval of pCu^{2+} predicted with WHAM VII when considering the analytical uncertainty on pH and total Cu and DOM concentrations (see Material and Methods section for rationale). Empty data points represent soil samples 18, 29, and 47 that were replicated thrice with their standard deviation as horizontal error bar. The thin solid line represents the regression line. The thick solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 0.5 pCu^{2+} unit. R^2_{adj} = adjusted R^2; *RMSR* = root mean square residual.

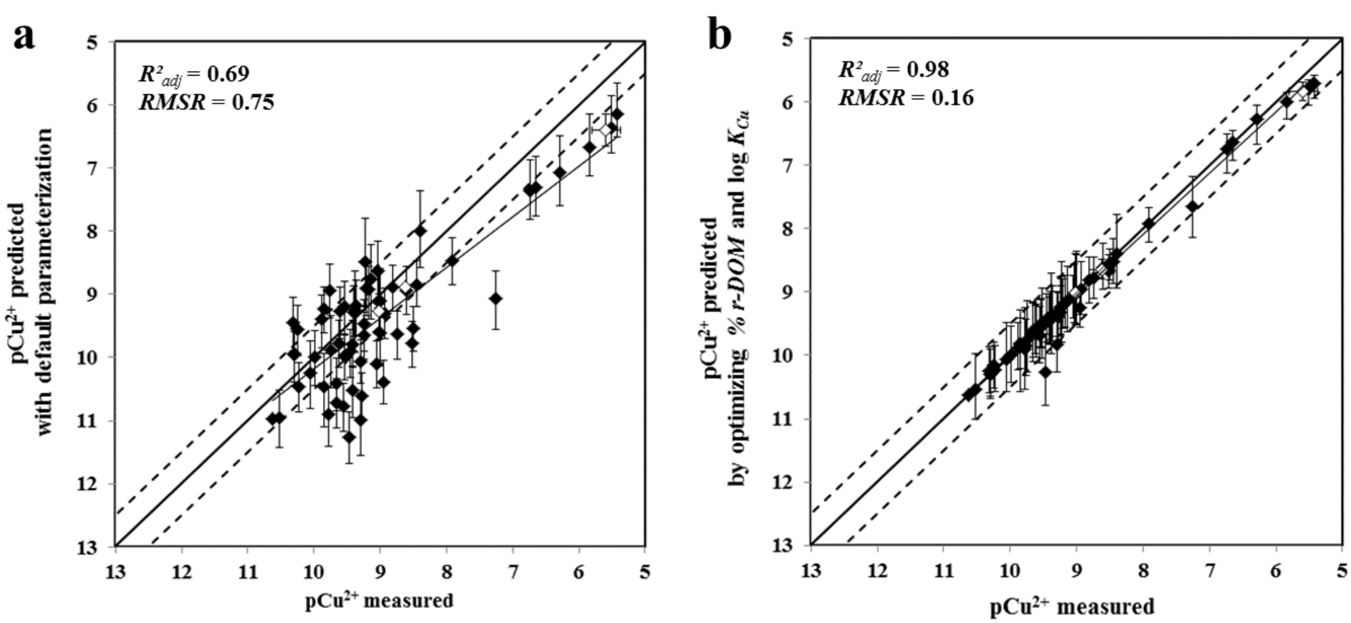

Figure S6. Free Cu activity (pCu^{2+}) predicted with WHAM VII as a function of the measured pCu^{2+} in the 55 soil solutions of experiments 4. Free Cu activity was predicted with WHAM VII by using either (a) a single, default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM* = 65 %), the Cu binding constant of reactive DOM ($\log K_{Cu}$ = 2.16), and the solubility constants of $Fe(OH)_3$ ($\log Ks_{Fe}$ = 2.7) and $Al(OH)_3$ ($\log Ks_{Al}$ = 8.5) for all solutions or (b) an optimized value of *% r-DOM* and $\log K_{Cu}$ within a range restricted to physically meaningful values for each soil solution. Vertical error bars represent the 95 % confident interval of pCu^{2+} predicted with WHAM VII when considering the analytical uncertainty on pH and total Cu and DOM concentrations (see Material and Methods section for rationale). Empty data points represent soil samples 18, 29, and 47 that were replicated thrice with their standard deviation as horizontal error bar. The thin solid line represents the regression line. The thick solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 0.5 pCu^{2+} unit. R^2_{adj} = adjusted R^2; *RMSR* = root mean square residual.

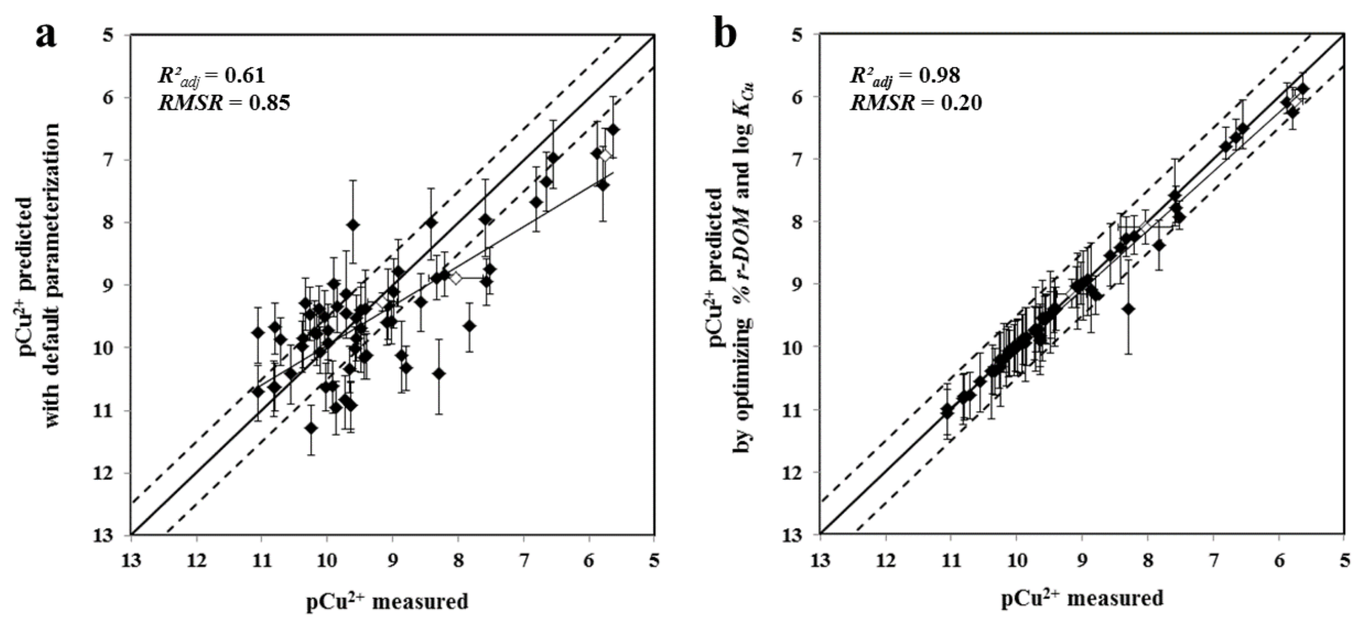

Figure S7. Toxic response (*R*) of plants (a and b), invertebrates (c and d) and microbial functions (e and f) calculated with FRIED model from pCu^{2+} predicted with WHAM VII (*y*-axis) or measured (*x*-axis) in the 55 soil solutions of experiments 2. The toxic endpoints are the growth of *Hordeum vulgare* roots (*Hv*, blue circles) and *Lycopersicon esculentum* shoots (*Le*, red circles) for plants, the reproduction of *Folsomia candida* (*Fc*, blue triangles) and *Eisenia fetida* (*Ef*, red triangles) for invertebrates, and the inhibition of potential nitrification (*PN*, blue squares), maize residue mineralization (*MRM*, red squares), and glucose-induced respiration (*GIR*, green squares) for microbial functions. *R* values of 100 and 0 represent the minimal and maximal toxicity of Cu, respectively. *R* values of 100 and 0 represent the minimal and maximal toxicity of Cu, respectively. Free Cu activity was predicted with WHAM VII by using either (a, c and e) a single, default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM* = 65 %), the Cu binding constant of reactive DOM (log K_{Cu} = 2.16), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe} = 2.7) and $Al(OH)_3$ (log Ks_{Al} = 8.5) for all solutions or (b, d and f) an optimized value of *% r-DOM* and log K_{Cu} within a range restricted to physically meaningful values for each soil solution. The error bars represent the standard deviation (n = 3) for soil samples 18, 29, and 47. The solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 10 %. *RMSR* = root mean square residual.

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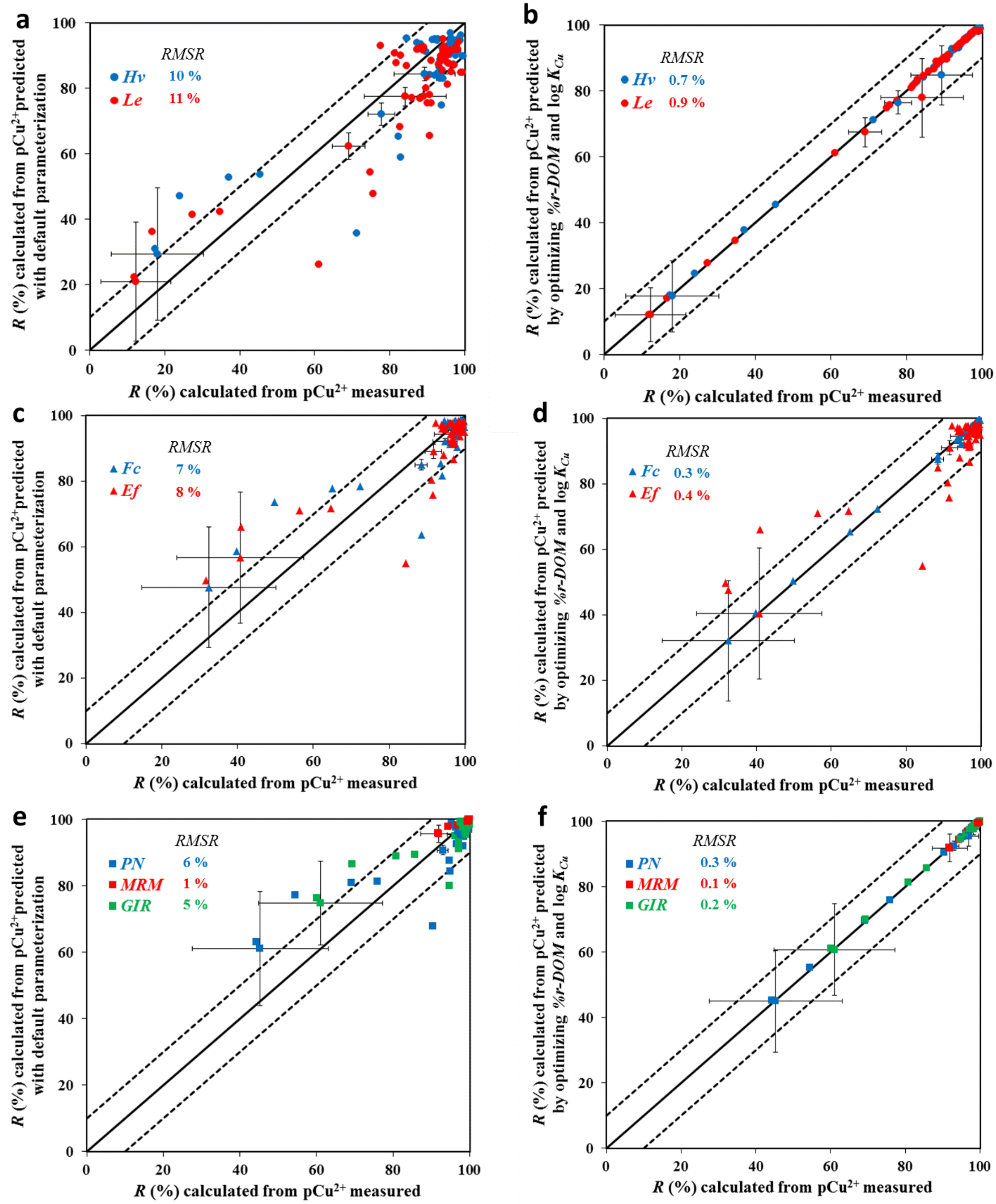

Figure S8. Toxic response (*R*) of plants (a and b), invertebrates (c and d) and microbial functions (e and f) calculated with FRIED model from pCu^{2+} predicted with WHAM VII (*y*-axis) or measured (*x*-axis) in the 55 soil solutions of experiments 3. The toxic endpoints are the growth of *Hordeum vulgare* roots (*Hv*, blue circles) and *Lycopersicon esculentum* shoots (*Le*, red circles) for plants, the reproduction of *Folsomia candida* (*Fc*, blue triangles) and *Eisenia fetida* (*Ef*, red triangles) for invertebrates, and the inhibition of potential nitrification (*PN*, blue squares), maize residue mineralization (*MRM*, red squares), and glucose-induced respiration (*GIR*, green squares) for microbial functions. *R* values of 100 and 0 represent the minimal and maximal toxicity of Cu, respectively. *R* values of 100 and 0 represent the minimal and maximal toxicity of Cu, respectively. Free Cu activity was predicted with WHAM VII by using either (a, c and e) a single, default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM* = 65 %), the Cu binding constant of reactive DOM (log K_{Cu} = 2.16), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe} = 2.7) and $Al(OH)_3$ (log Ks_{Al} = 8.5) for all solutions or (b, d and f) an optimized value of *% r-DOM* and log K_{Cu} within a range restricted to physically meaningful values for each soil solution. The error bars represent the standard deviation (n = 3) for soil samples 18, 29, and 47. The solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 10 %. *RMSR* = root mean square residual.

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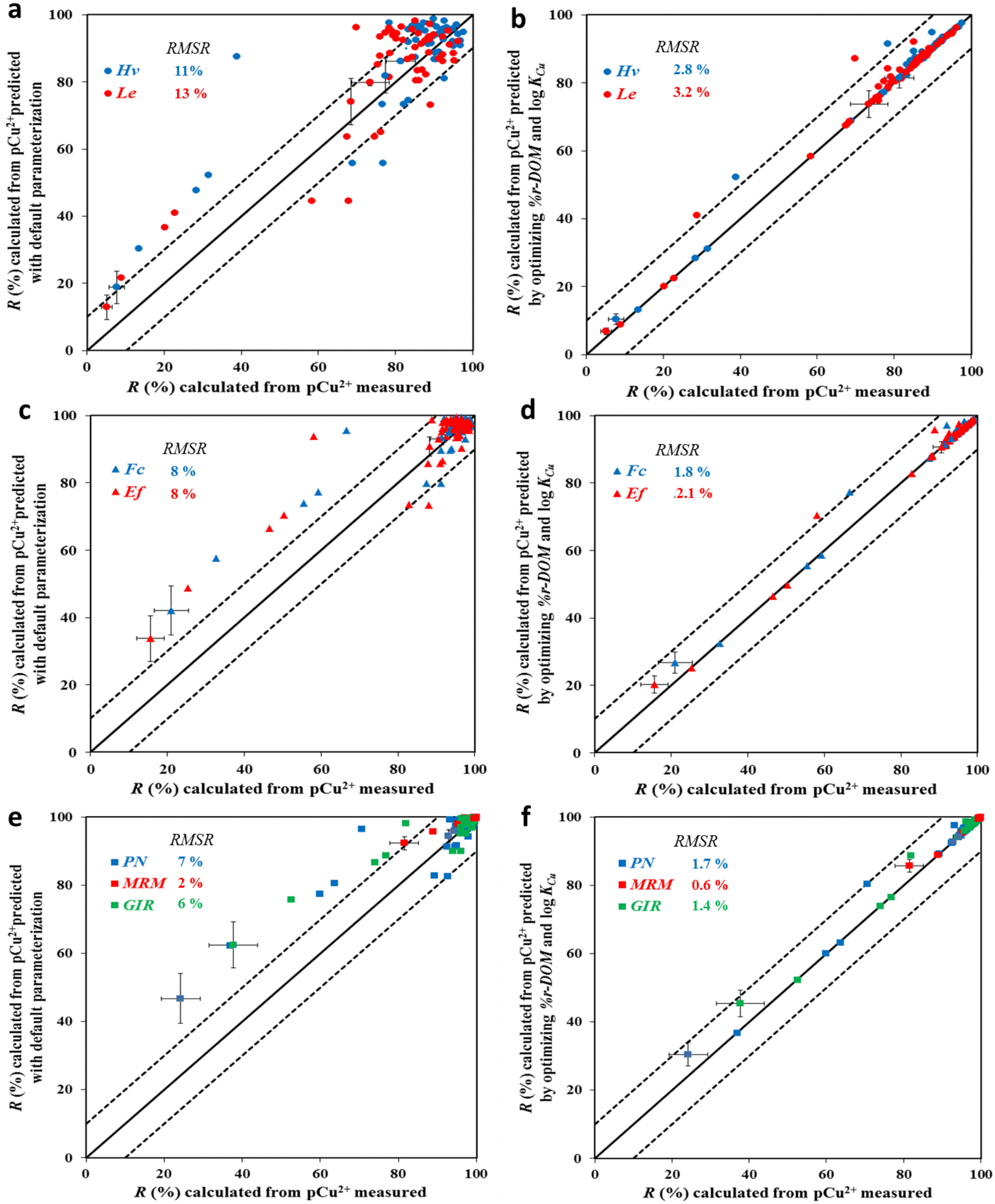

Figure S9. Toxic response (*R*) of plants (a and b), invertebrates (c and d) and microbial functions (e and f) calculated with FRIED model from pCu^{2+} predicted with WHAM VII (*y*-axis) or measured (*x*-axis) in the 55 soil solutions of experiments 4. The toxic endpoints are the growth of *Hordeum vulgare* roots (*Hv*, blue circles) and *Lycopersicon esculentum* shoots (*Le*, red circles) for plants, the reproduction of *Folsomia candida* (*Fc*, blue triangles) and *Eisenia fetida* (*Ef*, red triangles) for invertebrates, and the inhibition of potential nitrification (*PN*, blue squares), maize residue mineralization (*MRM*, red squares), and glucose-induced respiration (*GIR*, green squares) for microbial functions. *R* values of 100 and 0 represent the minimal and maximal toxicity of Cu, respectively. *R* values of 100 and 0 represent the minimal and maximal toxicity of Cu, respectively. Free Cu activity was predicted with WHAM VII by using either (a, c and e) a single, default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM* = 65 %), the Cu binding constant of reactive DOM (log K_{Cu} = 2.16), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe} = 2.7) and $Al(OH)_3$ (log Ks_{Al} = 8.5) for all solutions or (b, d and f) an optimized value of *% r-DOM* and log K_{Cu} within a range restricted to physically meaningful values for each soil solution. The error bars represent the standard deviation (*n* = 3) for soil samples 18, 29, and 47. The solid line represents the 1:1 line. Dashed lines represent the 1:1 line ± 10 %. *RMSR* = root mean square residual.

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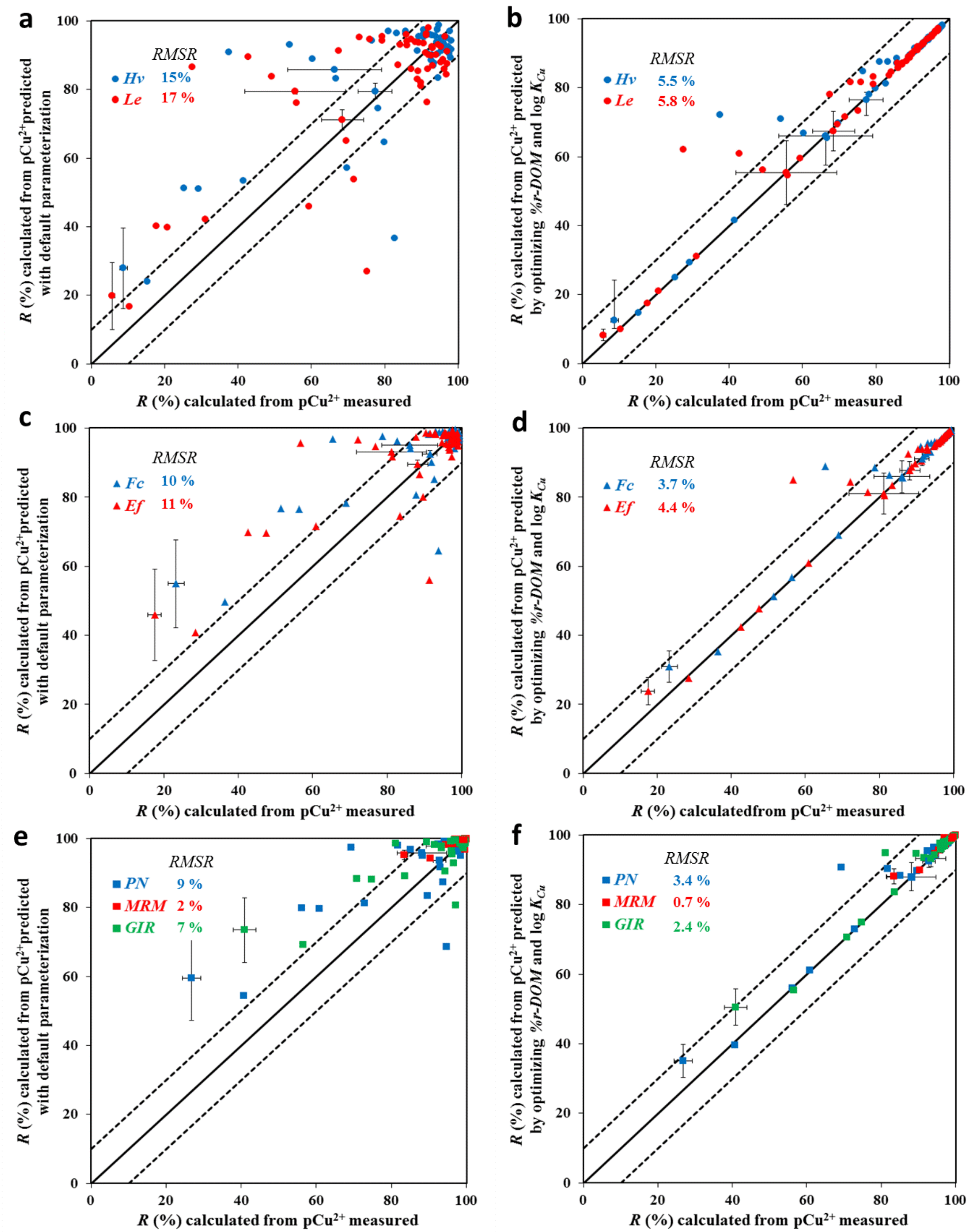

Table S9. Deviation calculated as the root mean square residual (*RMSR*) between measured and predicted free Cu^{2+} activities (pCu^{2+}) in the 55 soil solutions of experiment 2. Free Cu^{2+} activities were predicted with WHAM VII by using either a single default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM*), the Cu binding constant of reactive DOM (log K_{Cu}), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}) and $Al(OH)_3$ (log Ks_{Al}) for all soil solutions or an optimized value of *% r-DOM*, log K_{Cu}, log Ks_{Fe}, or log Ks_{Al} with or without restriction for each soil solution.

	pCu^{2+} predicted					
	pCu^{2+} modelling by default[a]		pCu^{2+} modelling with unrestricted optimization[b]		pCu^{2+} modelling with restricted optimization[c]	
	Parameters	pCu^{2+} *RMSR*	Parameters	pCu^{2+} *RMSR*	Parameters	pCu^{2+} *RMSR*
% r-DOM	65		0 to 5140	0.002	35 to 215[d]	0.41
Log K_{Cu}	2.16	0.83	≤ -1.53 to 2.87	0.08	1.84 to 2.46[e]	0.28
Log Ks_{Fe}	2.7		≤ -5.7 to 13.1	0.55	2.5 to 5[f]	0.74
Log Ks_{Al}	8.5		≤ 1.6 to 28.3	0.75	8.0 to 9.0[g]	0. 82
% r-DOM and Log K_{Cu}	-		-	-	35 to 215[d] and 1.84 to 2.46[e]	0.14

[a] Free Cu^{2+} was calculated by setting the four parameters at default values given by Model VII.

[b] Free Cu^{2+} was calculated by optimizing a single parameter within an unrestricted range of values, while the three other parameters were set at default values given by Model VII.

[c] Free Cu^{2+} was calculated by optimizing a single parameter within a range restricted to physically meaningful values, while the three other parameters were set at default values given by Model VII.

[d]According to Richie and Perdue*

[e] According to Tipping**

[f] According to Baes and Mesmer***

[g] According to Tipping****

*Ritchie JD, Perdue EM. 2003. Proton-binding study of standard and reference fulvic acids, humic acids, and natural organic matter. *Geochim Cosmochim Ac* 67:85-96.

** Tipping E. 1998. Humic Ion-Binding Model VI: An Improved Description of the Interactions of Protons and Metal Ions with Humic Substances. *Aquat Geochem* 4:3-47.

***Baes CF, Mesmer RE. 1976. *Hydrolysis of cations*. Wiley.

****Tipping E, Rey-Castro C, Bryan SE, Hamilton-Taylor J. 2002. Al(III) and Fe(III) binding by humic substances in freshwaters, and implications for trace metal speciation. *Geochim Cosmochim Ac* 66:3211-3224.

Table S10. Deviation calculated as the root mean square residual (*RMSR*) between measured and predicted free Cu^{2+} activities (pCu^{2+}) in the 55 soil solutions of experiment 3. Free Cu^{2+} activities were predicted with WHAM VII by using either a single default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM*), the Cu binding constant of reactive DOM (log K_{Cu}), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}) and $Al(OH)_3$ (log Ks_{Al}) for all soil solutions or an optimized value of *% r-DOM*, log K_{Cu}, log Ks_{Fe}, or log Ks_{Al} with or without restriction for each soil solution.

	pCu^{2+} predicted					
	pCu^{2+} modelling by default[a]		**pCu^{2+} modelling with unrestricted optimization[b]**		**pCu^{2+} modelling with restricted optimization[c]**	
	Parameters	pCu^{2+} *RMSR*	Parameters	pCu^{2+} *RMSR*	Parameters	pCu^{2+} *RMSR*
% r-DOM	65		0.8 to 340	0.03	35 to 215[d]	0.48
Log K_{Cu}	2.16	0.75	≤ -2.43 to 2.42	0.17	1.84 to 2.46[e]	0.28
Log Ks_{Fe}	2.7		≤ -7.3 to 8.1	0.15	2.5 to 5[f]	0.35
Log Ks_{Al}	8.5		≤ 2.1 to 20.9	0.26	8.0 to 9.0[g]	0.73
% r-DOM and Log K_{Cu}	-		-	-	35 to 215[d] and 1.84 to 2.46[e]	0.16

[a] Free Cu^{2+} was calculated by setting the four parameters at default values given by Model VII.

[b] Free Cu^{2+} was calculated by optimizing a single parameter within an unrestricted range of values, while the three other parameters were set at default values given by Model VII.

[c] Free Cu^{2+} was calculated by optimizing a single parameter within a range restricted to physically meaningful values, while the three other parameters were set at default values given by Model VII.

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***Baes CF, Mesmer RE. 1976. *Hydrolysis of cations*. Wiley.

****Tipping E, Rey-Castro C, Bryan SE, Hamilton-Taylor J. 2002. Al(III) and Fe(III) binding by humic substances in freshwaters, and implications for trace metal speciation. *Geochim Cosmochim Ac* 66:3211-3224.

Table S11. Deviation calculated as the root mean square residual (*RMSR*) between measured and predicted free Cu^{2+} activities (pCu^{2+}) in the 55 soil solutions of experiment 4. Free Cu^{2+} activities were predicted with WHAM VII by using either a single default value for the percentage of dissolved organic matter reactive towards metal cations (*% r-DOM*), the Cu binding constant of reactive DOM (log K_{Cu}), and the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}) and $Al(OH)_3$ (log Ks_{Al}) for all soil solutions or an optimized value of *% r-DOM*, log K_{Cu}, log Ks_{Fe}, or log Ks_{Al} with or without restriction for each soil solution.

	pCu^{2+} predicted					
	pCu^{2+} modelling by default[a]		**pCu^{2+} modelling with unrestricted optimization**[b]		**pCu^{2+} modelling with restricted optimization**[c]	
	Parameters	pCu^{2+} *RMSR*	Parameters	pCu^{2+} *RMSR*	Parameters	pCu^{2+} *RMSR*
% r-DOM	65		0 to 653	0.02	35 to 215[d]	0.51
Log K_{Cu}	2.16	0.85	≤-2.43 to 2.62	0.25	1.84 to 2.46[e]	0.35
Log Ks_{Fe}	2.7		≤ -6.3 to 12.2	0.31	2.5 to 5[f]	0.53
Log Ks_{Al}	8.5		≤ 1.6 to 17.9	0.43	8.0 to 9.0[g]	0.83
% r-DOM and Log K_{Cu}	-		-	-	35 to 215[d] and 1.84 to 2.46[e]	0.20

[a] Free Cu^{2+} was calculated by setting the four parameters at default values given by Model VII.

[b] Free Cu^{2+} was calculated by optimizing a single parameter within an unrestricted range of values, while the three other parameters were set at default values given by Model VII.

[c] Free Cu^{2+} was calculated by optimizing a single parameter within a range restricted to physically meaningful values, while the three other parameters were set at default values given by Model VII.

[d]According to Richie and Perdue*

[e] According to Tipping**

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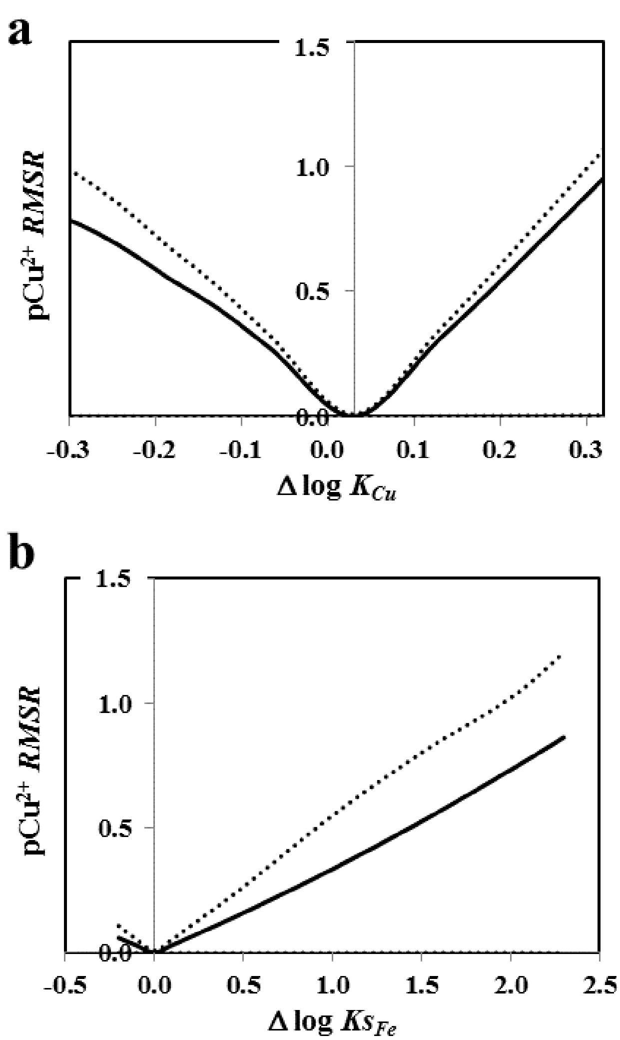
** Tipping E. 1998. Humic Ion-Binding Model VI: An Improved Description of the Interactions of Protons and Metal Ions with Humic Substances. *Aquat Geochem* 4:3-47.

***Baes CF, Mesmer RE. 1976. *Hydrolysis of cations*. Wiley.

****Tipping E, Rey-Castro C, Bryan SE, Hamilton-Taylor J. 2002. Al(III) and Fe(III) binding by humic substances in freshwaters, and implications for trace metal speciation. *Geochim Cosmochim Ac* 66:3211-3224.

Figure S10. Deviation in Cu^{2+} activity (pCu^{2+}) as a function of the variation in the Cu binding constant of reactive dissolved organic matter (log K_{Cu}, a), or the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}, b) or $Al(OH)_3$ (log Ks_{A}, c) in the 55 soil solutions of experiment 1 (see Table S6 for rationale on the range of variation in log K_{Cu}, log Ks_{Fe} ,and log Ks_{Al}). The solid curve represents the deviation expressed as the root mean square residual (*RMSR*) between pCu^{2+} measured and pCu^{2+} predicted in the 55 soil solutions with WHAM VII by using an optimized value of the percentage of dissolved organic matter reactive towards metal cations within an unrestricted range of values for each soil solution. Dashed lines represent the minimum and maximum deviation calculated for the corresponding soil solution.



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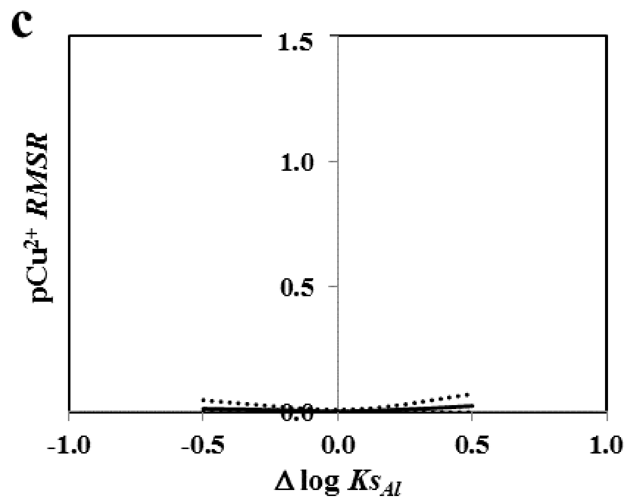

Figure S11. Deviation in Cu^{2+} activity (pCu^{2+}) as a function of the variation in the Cu binding constant of reactive dissolved organic matter (log K_{Cu}, a), or the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}, b) or $Al(OH)_3$ (log Ks_{A}, c) in the 55 soil solutions of experiment 2 (see Table S6 for rationale on the range of variation of log K_{Cu}, log Ks_{Fe} ,and log Ks_{Al}). The solid curve represents the deviation expressed as the root mean square residual (*RMSR*) between pCu^{2+} measured and pCu^{2+} predicted in the 55 soil solutions with WHAM VII by using an optimized value of the percentage of dissolved organic matter reactive towards metal cations within an unrestricted range of values for each soil solution. Dashed lines represent the minimum and maximum deviation calculated for the corresponding soil solution.

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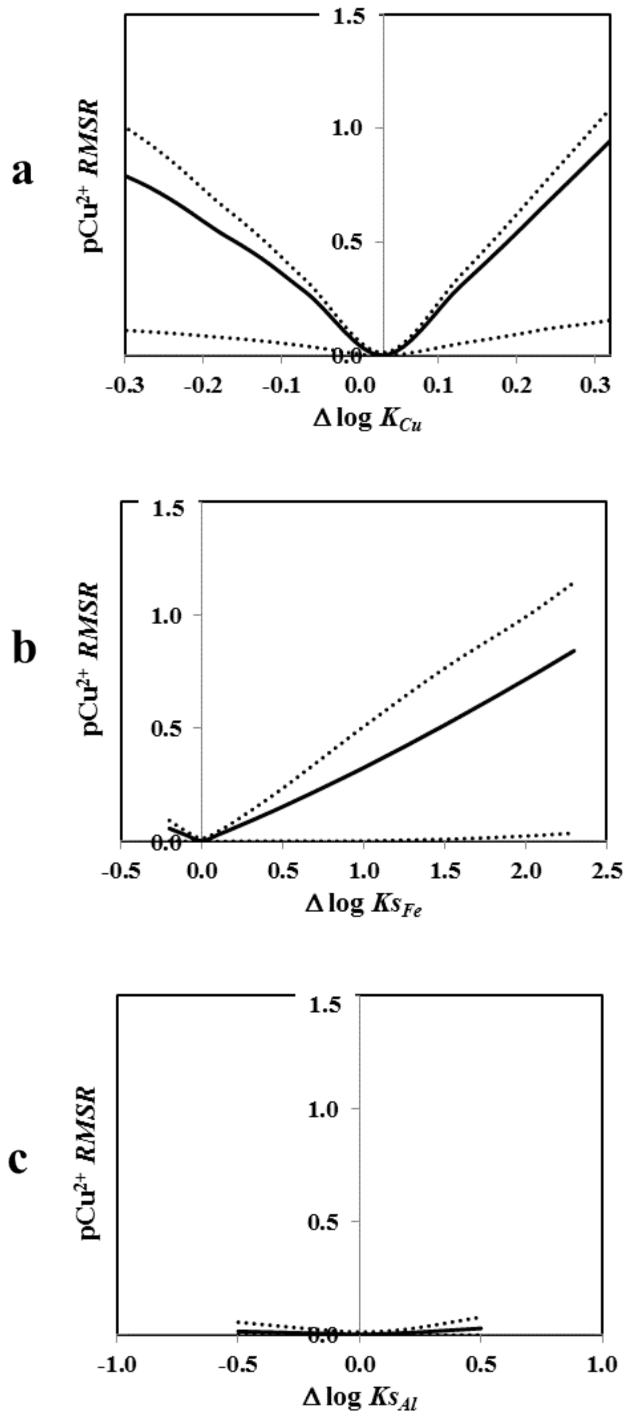
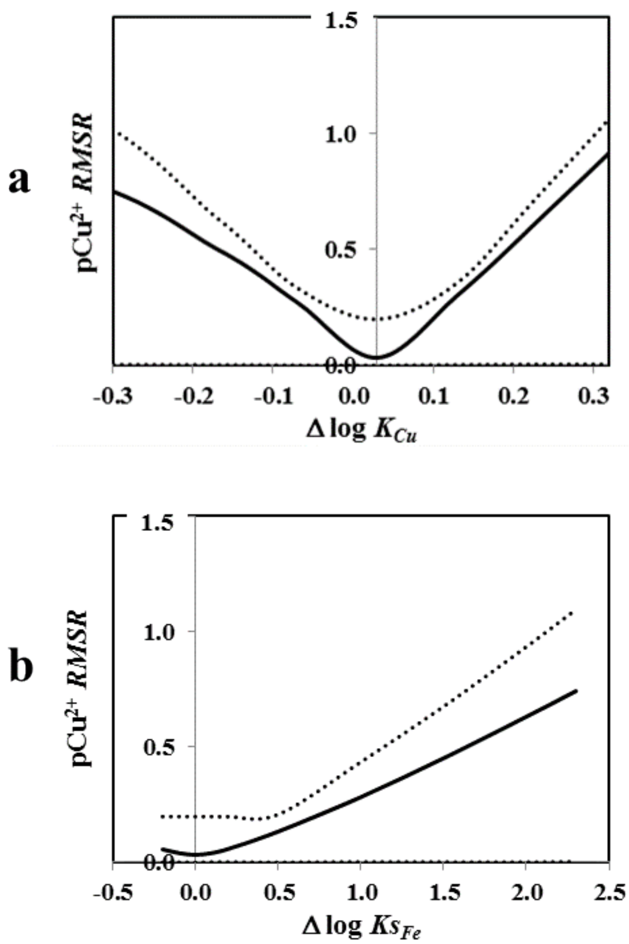


Figure S12. Deviation in Cu^{2+} activity (pCu^{2+}) as a function of the variation in the Cu binding constant of reactive dissolved organic matter (log K_{Cu}, a), or the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}, b) or $Al(OH)_3$ (log Ks_{A}, c) in the 55 soil solutions of experiment 3 (see Table S6 for rationale on the range of variation of log K_{Cu}, log Ks_{Fe} ,and log Ks_{Al}). The solid curve represents the deviation expressed as the root mean square residual (*RMSR*) between pCu^{2+} measured and pCu^{2+} predicted in the 55 soil solutions with WHAM VII by using an optimized value of the percentage of dissolved organic matter reactive towards metal cations within an unrestricted range of values for each soil solution. Dashed lines represent the minimum and maximum deviation calculated for the corresponding soil solution.



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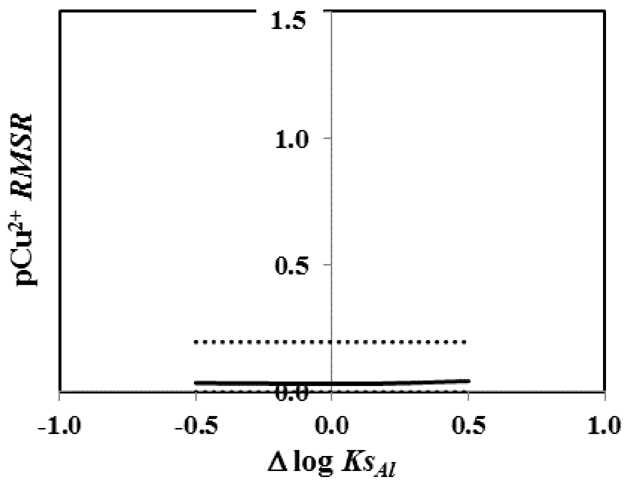

Figure S13. Deviation in Cu^{2+} activity (pCu^{2+}) as a function of the variation in the Cu binding constant of reactive dissolved organic matter (log K_{Cu}, a), or the solubility constants of $Fe(OH)_3$ (log Ks_{Fe}, b) or $Al(OH)_3$ (log Ks_{A}, c) in the 55 soil solutions of experiment 4 (see Table S6 for rationale on the range of variation of log K_{Cu}, log Ks_{Fe} ,and log Ks_{Al}). The solid curve represents the deviation expressed as the root mean square residual (*RMSR*) between pCu^{2+} measured and pCu^{2+} predicted in the 55 soil solutions with WHAM VII by using an optimized value of the percentage of dissolved organic matter reactive towards metal cations within an unrestricted range of values for each soil solution. Dashed lines represent the minimum and maximum deviation calculated for the corresponding soil solution.

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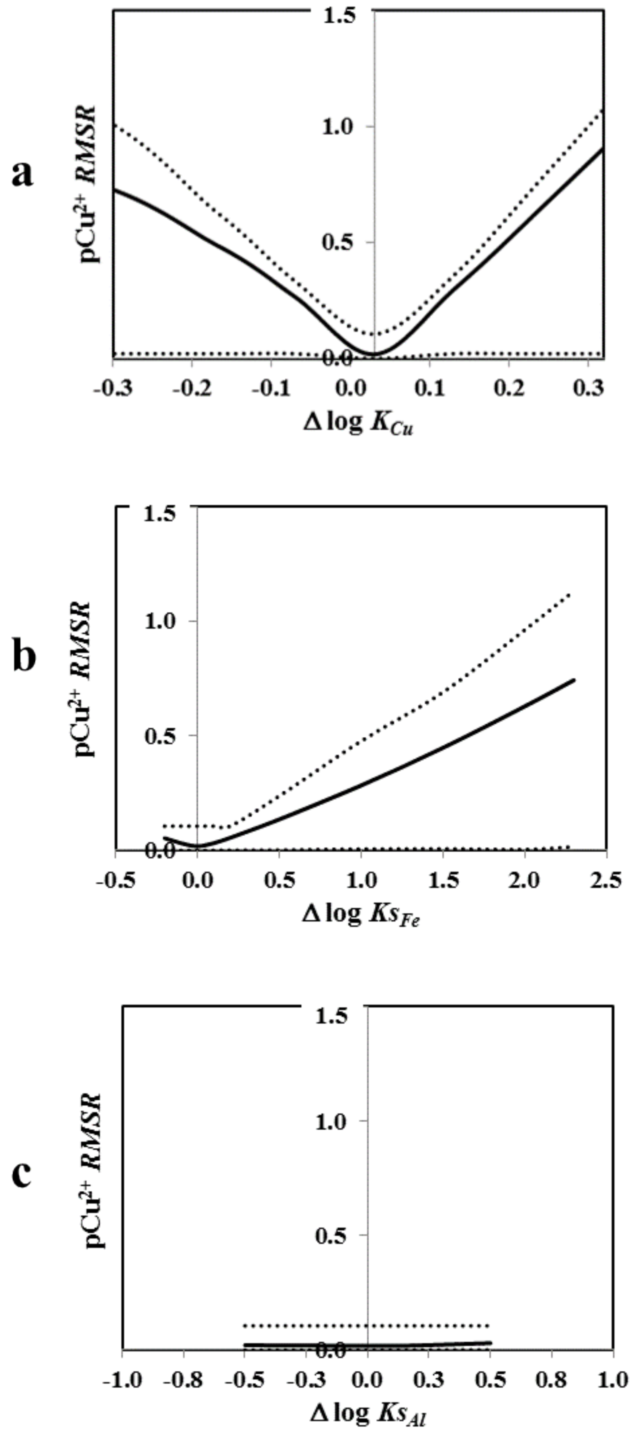

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